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Hartree-Fock Solutions Without Exchange for Normal Beryllium

Texas A&M University
College Station, Texas

[redacted]

PROGRESS REPORT TO THE NATIONAL AERONAUTICS

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Detailed Technical Supplement on Space Technology Project No. 5

(Hartree-Fock Solutions Without Exchange for Normal Beryllium)

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ABSTRACT

This is a first partial report on a study of the application of the Unrestricted Hartree-Fock scheme to the structure of atomic lithium. This report contains a detailed analysis of the application of the simpler Hartree-Fock equations without exchange to normal beryllium. Beryllium is the first non-trivial, general case of an atom with complete groups of electrons. The report develops the Hartree-Fock equations from first principles for beryllium and describes the numerical procedures employed to solve these equations. It contains flow diagrams and listings of the computer program along with instructions enabling a potential user to run the program. There is a first appendix giving a physical interpretation of the Hartree-Fock potentials followed by a second with tables and graphs of the radial wave functions computed by the program.

Author

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TABLE OF CONTENTS

DEFINITION OF TERMS

1. COMPLETE GROUPS OF ELECTRONS

The elements of the Slater determinants of many-body atomic theory are "so-called" one electron functions--solutions of certain single-particle central-field, wave equations. These wave equations involve the spherical harmonics $Y_{\ell m}$ as solutions of the angular parts of the Hamiltonian. For any fixed value of ℓ, there are $2\ell + 1$ spherical harmonics $Y_{\ell m}$ where m ranges through the set of values, $-\ell, -\ell + 1, \ldots, \ell - 1, \ell$. The set of one-electron wave functions corresponding to this collection of spherical harmonics is referred to as a complete group of electrons. The application of Slater determinants is generally much simpler when the one-electron functions of the determinants appear as complete groups of electrons.

2. CONFIGURATION

The simplest Hamiltonian H^1 for an N-electron atom is one in which each particle is assumed to move in an average central field due to the nucleus and the remaining (N-1)-electrons. The wave equation of the atom separates into a set of one-electron equations, each of which has eigensolutions determined by four quantum numbers; the principal quantum number n, the total angular momentum quantum number ℓ, the z-component of total angular momentum quantum number m_z, and the z-component of spin quantum number m_s. In this simple model, the Hamiltonian H^1 has no interaction terms depending upon the quantum numbers, m_z and m_s. Consequantly, any particular

eigenvalue of the energy operator H^1 corresponds to eigenfunctions which are the products of one-electron eigenfunctions with specified values for the principal quantum number n and the total angular momentum quantum number ℓ, independently of the values of the quantum numbers, m_z and m_s. A specification of these two quantum numbers, n and ℓ, for each of a set of N electrons is referred to as a configuration of the atom. Usually such a specification is made in terms of a code which we introduce later.

3. EQUATIONS WITH EXCHANGE

Hartree, Fock, and Slater have shown how to derive equations for many-particle systems by means of the variation principle. When the Pauli exclusion principle is taken into account through Slater determinants, such an application gives rise to the Hartree-Fock equations which are inhomogeneous in the one-electron, radial wave functions. The inhomogeneous part of the resulting equations can be described as resulting from "exhange of electrons" between the different one-electron wave functions. For this reason, these equations are called the equations with exchange.

4. EQUATIONS WITHOUT EXCHANGE

The equations resulting from the Hartree-Fock equations by omitting the exchange terms and those terms multiplied by off-diagonal parameters are referred to as the equations without exchange or sometimes as the Hartree equations.

5. EXCHANGE HOLE

According to the Hartree-Fock equations, each electron moves in the field of the nucleus, of all electrons of opposite spin, and in the field of a charge contribution of electrons of the same spin which is diminished, as a result of the exclusion principle, by a single unit of electronic charge. This sort of hole about the electron, resulting from the exclusion principle, is referred to as the exchange hole or the Fermi hole.

6. EXCHANGE POTENTIAL

The Hartree-Fock equations with exchange (see Definition 3) contain various potential-like terms which arise because of exchange properties of the one-electron wave functions. These terms constitute the exchange potential.

7. INCOMPLETE GROUPS OF ELECTRONS

A given configuration of an atomic system is said to contain an incomplete group of electrons if, for some n, not all possible one-electron wave functions for a given value of ℓ are in the configuration. The treatment of configurations containing incomplete groups is usually more difficult than those containing only complete groups.

8. LEVEL

The concept of level should be considered in the light of the definitions of configuration and term (see Definition 2 and Definition 19). For light atoms,

the central field Hamiltonian H^1 is usually improved by a perturbation interaction which includes the mutual Coulombic repulsion of the electrons to obtain an improved approximating Hamiltonian H^2. The symmetry group of H^2 is a proper subgroup of H^1 so that an energy eigenspace E^1 of H^1, a configuration, is usually the sum of several energy eigenspaces, $E^2_1, \ldots, E^2_n$, of H^2. A further improvement is obtained by including a coupling term between the orbital motion of an electron and its spin. This interaction is called spin-orbit coupling and its addition gives an approximating Hamiltonian H^3 whose symmetry group is a proper subgroup of that of H^2. As a consequence, an energy eigenspace E^2 of H^2, a term, is ordinarily the sum of several energy eigenspaces, $E^3_1, \ldots, E^3_n$, of the Hamiltonian H^3. These last eigenspaces, those of the approximating Hamiltonian H^3, are referred to as the levels of the system. In summary, the levels of an atomic system are those energy eigenspaces of an approximating Hamiltonian H^3 which includes both Coulombic repulsion between the electrons and spin-orbit interactions between the orbital motion and the spin of the electron.

9. QUANTUM NUMBER, PRINCIPAL

The time-independent Schrodinger's equation for a single particle, moving in a central field, when expressed in spherical polar coordinates separates into two parts, one of which involves the radial coordinate alone and the other involves the angular coordinates alone. This separation is

effected by means of a separation constant K which eventually must be so selected that the solutions of the equations satisfy certain physical conditions. The admissible values of K constitute one family of quantum numbers for the particle. Those that arise in this fashion are called the principal quantum numbers. They are intimately connected with the radial wave functions of the particle and, consequently, strongly influence the possible energy levels it may occupy.

10. QUANTUM NUMBER, SPIN

In the one-electron approach to the quantum mechanics of the N-electron atom, each electron is considered to have an existence of its own. In particular, each electron is specified by several quantum numbers, one of these is the spin quantum number which is supposed to define an internal degree of freedom of the electron.

11. QUANTUM NUMBER, TOTAL ORBITAL ANGULAR MOMENTUM

The total orbital angular momentum quantum number determine the value of the total orbital angular momentum of the single particle in the corresponding state, or else the total orbital angular momentum of some particular particle in the one-particle approach to the N-particle problem. See the two preceding definitions.

12. QUANTUM NUMBER, Z-COMPONENT OF TOTAL ORBITAL ANGULAR MOMENTUM (MAGNETIC QUANTUM NUMBER)

The projection of the total angular momentum along any direction is quantized either for the case of a single particle or for some particular particle in the one-particle approach to the many body problem. Conventionally, the axis selected is the z-axis and this z-component of total orbital angular momentum quantum number determines the value of this projection for the particular quantum state in question.

13. QUANTUM NUMBER, Z-COMPONENT OF SPIN

The z-component of spin quantum number is analogous, in the case of spin, to that defined in Definition 12 for total orbital angular momentum.

14. SCREENING NUMBER (CONSTANT)

The need to determine wave functions for unknown atoms from those of known atoms, leads to the introduction of various special parameters. One of these, the screening number (constant) is defined to be that number σ such that

$$R = R_{(H)}/(N - \sigma)$$

where R and $R_{(H)}$ are the mean radii of corresponding wave functions of an atom of atomic number N and of hydrogen, respectively. Thus we see that knowing (or having an estimate of) σ allows one to determine the mean radius of a wave function of an atom of atomic weight N from that of the corresponding

wave function of hydrogen. See Hartree, Calculation of Atomic Structures, pages 124-125, for further details. Unfortunately, like most numbers introduced for such a purpose, the screening constant is not a constant which seriously limits its value.

15. SLATER DETERMINANTS

Slater intoduced his famous "determinants" in the late twenties as trial functions for a determination of the wave function of an N-electron atom by means of the variation principle. The use of these determinants guarantees the observance of the Pauli exclusion principle in the solution so obtained. See page 6 of the following report.

16. SLATER INTEGRALS

The Slater Integrals occur in the systematic solution of the Hartree-Fock equations by use of Slater determinants when the one-electron functions are assumed to have a special form. See Hartree, Calculation of Atomic Structures, pages 45-50 for explicit definitions and further details.

17. SPIN QUANTUM NUMBER

See Definition 10.

18. STATE

The concept of state should be considered in the light of the definitions of configuration and level which are given in Definitions 2 and 8. Our observations in these definitions were that all of these concepts are related

through the degree of approximation assumed in the Hamiltonian H of an N-electron atom. The simplest Hamiltonian H^1 assumes that each electron of the atom moves in an averaged central field created by the nucleus and the other (N - 1) electrons. No direct interaction is assumed between the individual electrons. The energy eigenspaces arising for H^1 are called configurations. The next improved approximation is obtained by including in the Hamiltonian H^2 the Coulombic interaction between electrons. The energy eigenspaces of H^2 are called terms. A still better approximation for the N-electron atom is obtained by including a coupling in the Hamiltonian H^3 between the orbital motion of an electron and its spin. This interaction is sometimes called spin-orbit coupling. The energy eigenstates of H^3 are called levels. The final Hamiltonian H^4, in this sequence, includes a perturbation term from an external magnetic field. The eigenspaces of H^4 are called states and are one-dimensional invariant spaces of H^4, in general.

19. TERM

See Definitions 2, 8, and 18.

20. TOTAL ORBITAL ANGULAR MOMENTUM QUANTUM NUMBER

See Definition 11.

21. Y_k POTENTIAL

This function Y_k is related to the potential due to a single electron with total orbital angular momentum number k. See page 51, Hartree,

Calculation of Atomic Structures for greater detail.

22. Z-COMPONENT OF TOTAL ORBITAL ANGULAR MOMENTUM QUANTUM NUMBER

See Definition 12.

23. Z_k FIELD

This function Z_k is related to the field created by a single electron with total orbital angular momentum number k. See Hartree, Calculation of Atomic Structures, page 51.

SYMBOL LIST

$a_{(H)}$	The radius of the first Bohr orbit of the hydrogen atom taken to be the unit of length in our system of units.
$\|e\|$	The magnitude of the charge on the electron taken to be the unit of charge in our system.
$e^2/a_{(H)}$	The mutual potential energy of two unit charges at unit distance is taken to be the unit of energy. This unit is equal to twice the ionization energy of the normal state of the hydrogen atom.
f	One-electron wave function occurring in a Slater determinant.
h	Planck's constant which has a value of 2π in our system of units. This makes $\hbar = h/2\pi$ have the value of one.
H	The Hamiltonian of the atomic system under investigation.
m_e	The mass of the electron taken to have the value one in our system.
N	The number of electrons in the system, four in the case of normal beryllium.
0(x)	A symbol to denote that some function is asymptotic to x in some limiting process.
$P(n\ell; r)$	The "so-called" radial wave function of the electrons of the $(n\ell$th$)$-group.
r_i	The distance from the nucleus of the atom to the ith-electron of the system.
r_{ij}	The distance from the ith-electron of the system to the jth-electron.
u	Another symbol used for the one-electron functions which occur in the Slater determinant.
$\frac{Y_o(n\ell, n\ell; r)}{r}$	The potential created by the electrons of the $(n\ell$th$)$-shell.

$\frac{Y(n\ell;\, r)}{r}$	The effective potential acting on an electron of the $(n\ell$th$)$-shell.
$\frac{Y(r)}{r}$	The effective potential of the nucleus as screened by the surrounding cloud of electrons.
Z	The charge on the nucleus. The value of Z is different from that of N in the case of ionized atoms.
$\frac{Z_o(n\ell, n\ell;\, r)}{r^2}$	The field created by the electrons of the $(n\ell$th$)$-shell.
$\frac{Z(n\ell;\, r)}{r^2}$	The effective field of the nucleus acting on an electron of the $(n\ell$th$)$-shell.
$\frac{Z(r)}{r^2}$	The effective field of the nucleus as screened by the surrounding cloud of electrons.
δ_r	The increment in the independent variable r for numerical calculations. The value of δ_r varies during the calculation.
ϵ	This symbol is commonly used to denote an eigenvalue.
$\epsilon_{n\ell}$	This symbol is used to indicate certain parameters which arise during minimization of the energy. They are closely related to the energy values of the $(n\ell$th$)$-shell of the atom.
ψ	This symbol is used to denote the wave function of the system.

1. INTRODUCTION

This report is concerned with a detailed discussion of the determination of the wave functions of normal, atomic beryllium by means of the Hartree-Fock equations without exchange.

It should be pointed out that knowledge of the structure of atoms, parts of which can be obtained only by calculations of the type studied here, is essential to certain investigations of transition probabilities occurring in astrophysical studies, in problems in x-ray and neutron scattering, and, most important to us, in the calculation of the solid state wave functions of an element such as beryllium. The vital role played by studies in these areas and the limited number of people who are sufficiently familiar with these techniques to actually make a calculation have been the inspiration for this project.

A later report will concern itself with the Hartree-Fock equations including exchange, but a necessary preliminary step is the solution of the equations without exchange.

The present report is broken up into prefatory material, including definitions of terms and symbols; a body of twelve sections or paragraphs, the first six of which concern the theory and the last six the solutions of the Hartree-Fock equations; and two appendices which discuss and interpret the solutions.

In the case of beryllium, a solution Ψ of the wave equation is sought

in the form of a "so-called" Slater determinant; see page 6 for details. The individual entries in the determinant are called one-electron functions. The electrons in normal beryllium appear as four one-electron functions which are denoted by u_1, u_2, u_3, and u_4 in the Slater determinant. The possible forms of these functions are determined by a selection, a configuration, which is a prescription of the quantum numbers for total orbital angular momentum, z-component of orbital angular momentum, and the spin of the electrons which appear in the determinant. For beryllium, the configuration is described by the symbol $(1s)^2(2s)^2$.

Each of the one-electron functions is expressed in terms of polar co-ordinates and is taken to be the product of three functions: a function of r alone; a function of Θ and ϕ alone; and a function of spin alone. The second two factors of the one-electron functions are taken as given in the Hartree-Fock scheme. Thus the problem is limited to a determination of the "best" radial factors of the one-electron wave functions.

The units for calculations of this general nature are fairly standard. D. R. Hartree (1) gives an excellent discussion which we summarize briefly.

Unit of mass = m_e = rest mass of the electron

Unit of charge = $|e|$ = magnitude of the charge of the electron

Unit of length = $a_H = h^2/(4\pi^2 m_e |e|^2)$ = radius of the first Bohr orbit of the hydrogen atom

Consistently with these, we have

Unit of energy = $|e|^2/a_H$ = 2 x (ionization energy of the hydrogen atom)

Unit of velocity = $2\pi|e|^2/h = c/137$

This calculation is of a preliminary nature so that an effort was made to simplify the numerical analysis in order to get a running program as quickly as possible. Consequently, the present report is a description of a Hartree-Fock solution in which every numerical procedure is as simple as possible. The program has built-in, flexible tolerances throughout so that it is possible to get a rather good idea of the effects of various calculations on the over-all convergence of the problem. There is every indication that it may be worthwhile to use a very simple integration scheme in the initial stages of a Hartree-Fock calculation. The interested reader should look more closely at Section 11.

2. DEVELOPMENT OF THE FUNDAMENTAL EQUATIONS

We introduce the nomenclature and terminology to be used in discussing the application of the Hartree-Fock procedure to the normal beryllium atom. In the ground state, the beryllium atom is assumed to be in the configuration $(1s)^2(2s)^2$. This notation implies that two electrons have principal quantum number $n = 1$, total orbital angular momentum quantum number $\ell = 0$, magnetic quantum number $m_z = 0$ while one electron has spin quantum number $m_s = 1/2$ and the other $m_s = -1/2$. There are also two electrons with principal quantum number $n = 2$, total orbital angular momentum number $\ell = 0$, magnetic quantum number $m_z = 0$ while one has spin $m_s = 1/2$ and the other $m_s = -1/2$. We denote the single-particle wave functions for these electrons by f_1, f_2, f_3, and f_4.

Our first assumption is that these functions are products of three factors: the first is a function of the radial distance alone, the second of the angular variables alone, and the third of the spin alone. Furthermore, it is assumed that the angular and spin dependences of the functions are completely determined by the quantum numbers ℓ, m_z, and m_s

2-1
$$f_1 = P(10; r)\left[\theta_{00}(\theta)\Phi_0(\Phi)\right]\alpha$$
$$P(1s; r)$$
$$f_2 = P(10; r)\left[\theta_{00}(\theta)\Phi_0(\Phi)\right]\beta$$
$$P(1s; r)$$
$$f_3 = P(20; r)\left[\theta_{00}(\theta)\Phi_0(\Phi)\right]\alpha$$
$$P(2s; r)$$
$$f_4 = P(20; r)\left[\theta_{00}(\theta)\Phi_0(\Phi)\right]\beta$$
$$P(2s; r)$$

where $P(n\ell; r)$ denotes the radial function corresponding to the quantum numbers n (principal) and ℓ(total orbital angular); θ_{ℓ_m} is the associated Legendre function corresponding to the quantum number ℓ(total orbital angular momentum) and m_z (magnetic), while $\Phi_m(\Phi)$ denotes the azimuthal function depending on m_z alone. We list a few members of this family of functions for convenience and concreteness

2-2
$$\Phi_0(\Phi) = \frac{1}{\sqrt{2\pi}}$$
$$\Phi_1(\Phi) = \frac{e^{i(\Phi)}}{\sqrt{2\pi}}$$

$$\theta_{00}(\theta) = \frac{\sqrt{2}}{2}$$

$$\theta_{10}(\theta) = \frac{\sqrt{6}\cos\theta}{2}$$

$$\theta_{1\pm1}(\theta) = \frac{\sqrt{3}\sin\theta}{2}$$

The numerical constants in these functions have been so selected that

2-3
$$\int_0^{2\pi} \Phi_m^* \Phi_m \, d\phi = 1$$

$$\int_0^{\pi} \left[\theta_{\ell m}(\theta)\right]^2 \sin\theta \, d\theta = 1$$

Our basic problem is to determine the radial functions P(10; r) $\left[= P(1s; r)\right]$ and P(20; r) $\left[=P(2s; r)\right]$ for beryllium. The Hartree-Fock procedure is a particular method for doing this.

Hartree originally selected a best wave function in a somewhat heuristic manner from the set of all wave functions of the form

$$u_1(1)u_2(2)u_3(3)u_4(4)$$

Basically his method is to consider each electron moving in an average field produced by the other electrons. Slater and Fock discovered independently that a more general technique based on a variation principal led to a set of equations quite similar to Hartree's. Furthermore, by applying the variation procedure to a specially constructed set of functions, it is possible to satisfy the symmetry requirements of Pauli's exclusion principal. Such a wave function is one of the form

2-4
$$\Psi = \frac{1}{\sqrt{4!}} \sum_{P \in S_4} \delta_P P\left[u_1(1)u_2(2)u_3(3)u_4(4)\right]$$

where P runs through the set of all permutations of S_4, in the case of a four-particle system such as beryllium, and $\delta_P = 1$ or $\delta_P = -1$ according to whether P is an even or an odd permutation.

Our notation $u_i(j)$ is a description of the event that particle or electron j is in a state described by the single particle wave function u_i. Recall that the action of the permutation operator P, or more properly O_P, upon such a wave function is given by

2-5
$$O_P\left[u_i(j)\right] = u_i\left[P^{-1}(j)\right]$$

The function Ψ is more commonly written in the form of a Slater determinant.

2-6
$$\Psi = \frac{1}{\sqrt{4!}} \begin{vmatrix} u_1(1)u_1(2)u_1(3)u_1(4) \\ u_2(1)u_2(2)u_2(3)u_2(4) \\ u_3(1)u_3(2)u_3(3)u_3(4) \\ u_4(1)u_4(2)u_4(3)u_4(4) \end{vmatrix}$$

We wish to specialize ψ to the case where the functions u_1, u_2, and so on, have the form f_1, f_2, f_3, and f_4; functions having prescribed spin and angular characteristics with only the radial dependence to be determined, that is, P(10; r) and P(20; r) are the unknown functions.

The Hartree-Fock equations are the conditions which must be satisfied by the functions $P(n_\ell\ ;\ r)$ in order that the quantity

2-7
$$E' = \int \Psi^* H \Psi d\tau \Big/ \int \Psi^* \Psi d\tau$$

is stationary with respect to variations in these radial wave functions.

In order to find the equations, we must first determine E' and then the conditions on $P(n\ell; r)$ which make E' stationary. The usual Hamiltonian for an N electron atom in which the nucleus is taken as a fixed center is of the form

2-8
$$(-\hbar^2/8\pi^2 m_e)\sum_{j=1}^{N}\nabla^2_j - \sum_{j=1}^{N} Ze^2/r_j + \sum_{\substack{j=1\\ i>j}}^{N} e^2/r_{ji}$$

where the notation $\sum_{\substack{j=1\\ i>j}}^{N} e^2/r_{ji}$ means sum all combinations of

j and i exactly once and Z denotes the charge on the neucleus (not the atomic number when the atom is assumed to be ionized). We are using a system of units in which $m_e = |e| = h^2/(4\pi^2 m_e) = 1$, so that the Hamiltonian for beryllium is H =

2-9
$$-(1/2)\sum_{j=1}^{4}\nabla\left\{\nabla^2_j + 3/r_j\right\} + \sum_{\substack{j=1\\ i>j}}^{4} 1/r_{ji} =$$

$$(-1/2)\nabla^2_1 \; -4/r_1 \; +(1/2)\left\{1/r_{12} + 1/r_{13} + 1/r_{14}\right\}+$$
$$(-1/2)\nabla^2_2 \; -4/r_2 \; +(1/2)\left\{1/r_{21} + 1/r_{23} + 1/r_{24}\right\}+$$
$$(-1/2)\nabla^2_3 \; -4/r_3 \; +(1/2)\left\{1/r_{31} + 1/r_{32} + 1/r_{34}\right\}+$$
$$(-1/2)\nabla^2_4 \; -4/r_4 \; +(1/2)\left\{1/r_{41} + 1/r_{42} + 1/r_{43}\right\}$$

With each particle of an N particle quantum mechanical system Q we associate a three-dimensional co-ordinate space and a two-point spin space. All of these together give rise to a 3N-dimensional co-ordinate space E and a 2N-point spin space S of the system Q. The configuration

space C of Q is the cartesian product space E x S. We take the Lebesgue measure on E and the measure of each point of S to be one; then C is a measure space under the standard product measure.

The symbol $\int f d\tau$ denotes an integral over the entire configuration space arising from this product measure. If rectangular co-ordinates are introduced into E in the natural way, then $\int f d\tau =$

2-10 $$\sum\int f dx_1 dy_1 dz_1 \ldots dx_N dy_N dz_N$$

where $\sum$ denotes a sum over the points of spin space.

We may think of the points in S as labeled 1_α, 1_β, 2_α, 2_β, ... N_α, N_β so that

2-11 $$S = \left\{1_\alpha,\ 1_\beta,\ \ldots,\ N_\alpha,\ N_\beta\right\}$$

The spin functions $\alpha(i)$ and $\beta(i)$ are associated with the spin space $\left\{ i_\alpha,\ i_\beta \right\}$ of the ith particle with the function $\alpha(i)$ having the value one at i_α and the value zero at i_β and the function $\beta(i)$ having the value zero at i_α and the value one at i_β. When a function f is the product of N single particle functions, the spin factor of f is the product $\gamma(1)\gamma(2)\ldots\gamma(n)$ where each factor $\gamma(i)$ is either $\alpha(i)$ or $\beta(i)$. We note that $\alpha(i)$ and $\beta(i)$ are orthonormal in the sense that $\int\alpha(i)\beta(i) = \alpha(i_\alpha)\beta(i_\alpha) + \alpha(i_\beta)\beta(i_\beta) = 0$ and, similarly, $\int\gamma(i)^2 = 1$.

We restrict our attention to a four particle system appropriate to beryllium. Consider two functions f and g which are products, $f = f_1 f_2 f_3 f_4$ and $g = g_1 g_2 g_3 g_4$, of single particle functions with $f_i = f_i'\gamma(i)$ and $g_i = g_i'\delta(i)$ where f_i' and g_i' are spatial functions and $\gamma(i)$ and $\delta(i)$ are spin functions equal to one or the other

of the functions $\alpha(i)$ or $\beta(i)$. The integral $\int f^* g \, d\tau$ =

2-12
$$\int f_1^* g_1 f_2^* g_2 f_3^* g_3 f_4^* g_4 d\tau =$$
$$\left[\sum \gamma(1)\delta(1)\gamma(2)\delta(2)\gamma(3)\delta(3)\gamma(4)\delta(4)\right] \times$$
$$\left[\int f_1'^* g_1' dx_1 dy_1 dz_1\right] \times$$
$$\cdots$$
$$\left[\int f_4'^* g_4' dx_4 dy_4 dz_4\right] =$$
$$\left[\sum \gamma(1)\delta(1)\right] \times \cdots \times \left[\sum \gamma(4)\delta(4)\right] \times$$
$$\left[\int f_1'^* g_1' dx_1 dy_1 dz_1\right] \times \cdots \times \left[\int f_4'^* g_4' dx_4 dy_4 dz_4\right]$$

We observe that the factor $\left[\sum \gamma(i)\delta(i)\right]$ is zero unless $\gamma(i) = \delta(i) = \alpha(i)$ or $\gamma(i) = \delta(i) = \beta(i)$. Thus the integral $\int f^* g \, d\tau$ is zero unless the spin functions of factors of f <u>match</u> with the spin functions of the factors of g.

Furthermore if the sets $\{f_1', f_2', f_3', f_4'\}$ and $\{g_1', g_2', g_3', g_4'\}$ are rearrangements or permutations of the orthonormal set $\{u_1', u_2', u_3', u_4'\}$ of functions, then

2-13
$$\int f_i'^* g_i' dx_i dy_i dz_i$$

is one if and only if the functions f and g coincide, otherwise it is zero. We see that $\int f^* g \, d\tau$ is zero, in this case, unless both the corresponding spatial and the spin factors match. These orthogonality properties are crucial for our development of the Hartree-Fock equations.

These results may be presented in another form if we let $d\tau_1$, $d\tau_2$, $d\tau_3$, and $d\tau_4$ be the <u>volume elements</u> associated with both the spatial and spin co-ordinates of particles one, two, three, and four. Then $\int f^* g \, d\tau$ =

2-14
$$\int f_1^* g_1 d\tau_1 \int f_2^* g_2 d\tau_2 \int f_3^* g_3 d\tau_3 \int f_4^* g_4 d\tau_4$$

and, when the f's and g's are permutations of the same set of functions, orthonormal over both spatial and spin co-ordinates, the integral is zero unless $f_i = g_i$, $1 \leq i \leq 4$.

There is a slight variation on this theme when g is operated on by a linear transformation T affecting only those factors of g which are functions of certain co-ordinates. For example, let $Th = x_1x_2h$ for any function h defined on the configuration space C. In this case,

2-15 $$\int f^*Tg\, d\tau =$$
$$\int f_1^*x_1g_1 d\tau \int f_2^*x_2g_2 d\tau \int f_3^*g_3 d\tau \int f_4^*g_4 d\tau$$

If the f's and g's are permutations of an orthonormal set, then f_3 must equal g_3 and f_4 must equal g_4 in order that $\int f^*g\, d\tau$ be different from zero. However, the presence of x_1 and x_2 in the first two factors ordinarily destroys orthogonality and it is no longer necessary that f_1 be equal to g_1 and f_2 be equal to g_2.

This observation is pertinent to the evaluation of the integrals $\int \psi^*\psi d\tau$ and $\int \psi^*H\psi d\tau$ where ψ is the Slater determinent

2-16 $$\psi = \sum_{P \in S_4} \delta_P Pf_1(1)f_2(2)f_3(3)f_4(4)$$

We begin with an observation on the change of variable in certain related integrals. Let P and Q denote any two elements of S_4 where

2-17 $$P^{-1} = \begin{pmatrix} 1 & 2 & 3 & 4 \\ P_1 & P_2 & P_3 & P_4 \end{pmatrix}, \text{ and}$$
$$Q^{-1} = \begin{pmatrix} 1 & 2 & 3 & 4 \\ q_1 & q_2 & q_3 & q_4 \end{pmatrix}$$

From these definitions, it follows that

2-18 $$P\left[f_1^*(1)f_2^*(2)f_3^*(3)f_4^*(4)\right] = f_1^*(p_1)f_2^*(p_2)f_3^*(p_3)f_4^*(p_4), \text{ and}$$
$$Q\left[f_1(1)f_2(2)f_3(3)f_4(4)\right] = f_1(q_1)f_2(q_2)f_3(q_3)f_4(q_4).$$

Actually, in the above statements, the symbols P and Q are being used as a substitute for the more precise symbols, O_P and O_Q.

In the integral

2-19 $$\int\left\{P\left[f_1^*(1) \ldots f_4^*(4)\right]\right\}\left\{Q\left[f_1(1) \ldots f_4(4)\right]\right\}d\tau.$$

We make the change of variable x_1 going into x_{q_1}, x_2 going into x_{q_2}, x_3 going into x_{q_3}, and x_4 going into x_{q_4}. Actually, we are considering this as merely a change of name of the variable of integration. The following relations follow from such a name change.

2-20 $$\int\left\{P\left[f_1^*(1)f_2^*(2)f_3^*(3)f_4^*(4)\right]\right\}\left\{Q\left[f_1(1)f_2(2)f_3(3)f_4(4)\right]\right\}d\tau =$$
$$\int\left\{Q^{-1}P\left[f_1^*(1)f_2^*(2)f_3^*(3)f_4^*(4)\right]\right\}\left\{Q^{-1}Q\left[f_1(1)f_2(2)f_3(3)f_4(4)\right]\right\} =$$
$$\int\left\{Q^{-1}P\left[f_1^*(1)f_2^*(2)f_3^*(3)f_4^*(4)\right]\right\}\left\{f_1(1)f_2(2)f_3(3)f_4(4)\right\}d\tau =$$
$$\int f_1^*(t_1)f_2^*(t_2)f_3^*(t_3)f_4^*(t_4)f_1(1)f_2(2)f_3(3)f_4(4)d\tau$$

where $\left[PQ^{-1}\right](1) = t_1$, $\left[PQ^{-1}\right](2) = t_2$, $\left[PQ^{-1}\right](3) = t_3$, and $\left[PQ^{-1}\right](4) = t_4$. We may rearrange the factors in this integral such that variable one occurs in the first factor, variable two in the second factor, and so on, that is, according to the permutation $\left[QP^{-1}\right]$ where $\left[QP^{-1}\right](1) = r_1$, $\left[QP^{-1}\right](2) = r_2$, $\left[QP^{-1}\right](3) = r_3$, $\left[QP^{-1}\right](4) = r_4$. With this rearrangement, the integral becomes

2-21

$$\int f_{r_1}^*(1) f_{r_2}^*(2) f_{r_3}^*(3) f_{r_4}^*(4) f_1(1) f_2(2) f_3(3) f_4(4) d\tau = \int f_{r_1}^* f_1 d\tau_1 \int f_{r_2}^* f_2 d\tau_2 \int f_{r_3} f_3 d\tau_3 \int f_{r_4} f_4 d\tau_4$$

We observe that at least one factor of this product is zero unless QP^{-1} is the identity permutation, that is, unless Q = P. In this last instance

2-22 $$\int f_1^* f_2^* f_3^* f_4^* f_1 f_2 f_3 f_4 d\tau = 1$$

We now consider the integral $\int \psi^* \psi d\tau$ where

2-23 $$\psi^* = \sum_{P \epsilon S_4} \delta_P P\left[f_1^* f_2^* f_3^* f_4^*\right] \text{ and}$$

$$\psi = \sum_{Q \epsilon S_4} \delta_Q Q\left[f_1 f_2 f_3 f_4\right] .$$

Then

2-24 $$\int \psi^* \psi d\tau =$$

$$\int \sum_{P \epsilon S_4} \delta_P P\left[f_1^* f_2^* f_3^* f_4^*\right] \sum_{Q \epsilon S_4} \delta_Q Q\left[f_1 f_2 f_3 f_4\right] d\tau =$$

$$\sum_{P \epsilon S_4} \delta_P \sum_{Q \epsilon S_4} \delta_Q \int \left\{P\left[f_1^* f_2^* f_3^* f_4^*\right]\right\}\left\{Q\left[f_1 f_2 f_3 f_4\right]\right\} d\tau =$$

$$\sum_{P \epsilon S_4} \delta_P \sum_{Q \epsilon S_4} \delta_Q \int \left\{Q^{-1} P\left[f_1^* f_2^* f_3^* f_4^*\right]\right\}\left\{f_1 f_2 f_3 f_4\right\} d\tau =$$

$$\sum_{P \epsilon S_4} \delta_P \delta_P \int \left\{P^{-1} P\left[f_1^* f_2^* f_3^* f_4^*\right]\right\}\left\{f_1 f_2 f_3 f_4\right\} d\tau = 24$$

The next problem is to evaluate the expression $\int \psi^* H \psi d\tau$. This integral can be written as the sum of four terms of which we consider only the first in detail

2-25 $$\int \psi^* H \psi d\tau =$$

$$(-1/2) \int \psi^* \left\{\nabla_1^2 + 8/r_1 - \left[1/r_{12} + 1/r_{13} + 1/r_{14}\right]\right\} \psi d\tau$$

$$+ \text{ Three other similar terms}$$

Ignoring the factor (-1/2), the first term is of the form

2-26 a) $\int \psi^* \nabla_1^2 \psi d\tau$ +

b) $8\int \psi^* (1/r_1)\psi d\tau$ -

c) $\int \psi^* (1/r_{12})\psi d\tau$ -

d) $\int \psi^* (1/r_{13})\psi d\tau$ -

e) $\int \psi^* (1/r_{14})\psi d\tau$

A typical term in the expansion of $\int \psi^* \nabla_1^2 \psi d\tau$ is

2-27 $$\int f_{P_1}^*(1) f_{P_2}^*(2) f_{P_3}^*(3) f_{P_4}^*(4) \nabla_1^2 f_{q_1}(1) f_{q_2}(2) f_{q_3}(3) f_{q_4}(4) d\tau =$$
$$\int f_{P_2}^* f_{q_2} d\tau_2 \int f_{P_3}^* f_{q_3} d\tau_3 \int f_{P_4}^* f_{q_4} d\tau_4 \int f_{P_1}^* \nabla_1^2 f_{q_1} d\tau_1$$

which is zero unless $P_2 = q_2$; $P_3 = q_3$; and $P_4 = q_4$. However, for a fixed value of $P_1 = q_1$, there are six distinct permutations of the remaining indices which fit this criterion. Thus we see that Part a) gives rise to the terms

2-28 $$6\left[\int f_1^*(1)\nabla_1^2 f_1(1)d\tau_1 + \int f_2^*(1)\nabla_1^2 f_2(1)d\tau_2 + \int f_3^*(1)\nabla_1^2 f_3(1)d\tau_3 + \int f_4^*(1)\nabla_1^2 f_4(1)d\tau_4\right]$$

2-29 $$\nabla_1^2 f_1 = \nabla_1^2 P(10; r)\theta_{00}\Phi_0\alpha =$$
$$\left[\frac{1}{r_1^2}\left(\frac{\partial}{\partial r_1} r_1^2 \frac{\partial}{\partial r_1}\right) + \frac{1}{r_1^2 \sin\theta_1}\left(\frac{\partial}{\partial\theta_1}\sin\theta_1 \frac{\partial}{\partial\theta_1}\right) + \frac{1}{r_1^2}\frac{1}{\sin^2\theta_1}\frac{\partial^2}{\partial\Phi_1^2}\right] P(10; r)\theta_{00}\Phi_0\alpha =$$
$$\theta_{00}\Phi_0\alpha\left[\frac{1}{r_1^2}\frac{\partial}{\partial r_1} r_1^2 \frac{\partial}{\partial r_1}\right] P(10; r) =$$
$$\theta_{00}\Phi_0\alpha\left[d^2/dr^2 + (2/r)d/dr\right]P(10; r)$$

2-30 $$\nabla_1^2 f_2 =$$
$$\nabla_1^2 P(10; r)\theta_{00}\Phi_0\beta =$$
$$\theta_{00}\Phi_0\beta\left[d^2/dr^2 + (2/r)d/dr\right]P(10; r)$$

2-31 $$\nabla_1^2 f_3 = \nabla_1^2 P(20; r)\theta_{00}\Phi_0\alpha =$$
$$\theta_{00}\Phi_0\alpha\left[d^2/dr^2 + (2/r)d/dr\right]P(20; r)$$

2-32 $\nabla_1^2 f_4 = \nabla_1^2 P(2\ell; r)\theta_{00}\Phi_0\beta =$

$\theta_{00}\Phi_0\beta\left[d^2/dr^2 + (2/r)d/dr\right]P(2\ell; r)$

We now observe, since the variable of integration is a matter of indifference, that

2-33 $\int f_1^*(1)\nabla_1^2 f_1(1)d\tau_1 =$

$\int f_1^*(2)\nabla_2^2 f_1(2)d\tau_2 =$

$\int f_1^*(3)\nabla_3^2 f_1(3)d\tau_3 =$

$\int f_1^*(4)\nabla_4^2 f_1(4)d\tau_4 =$

$$\int_0^\infty\int_0^\pi\int_0^{2\pi}\left[\theta_{00}\Phi_0\alpha\right]^2 P(10; r)\left\{\nabla^2 P(10; r)\right\}r^2\sin\theta\, d\Phi\, d\theta\, dr =$$

$$\int_0^\infty P(10; r)\left\{\nabla^2 P(10; r)\right\}r^2 dr$$

When f is a function of r alone, it is permissible to write $\nabla^2 f = (1/r)(d^2(rf)/dr^2)$. Thus the above integral may be written

2-34 $$\int_0^\infty P(10;r)\left\{(1/r)d^2(rP(10;r))/dr^2\right\}r^2 dr =$$

$$\int_0^\infty\left\{rP(10;r)\right\}\left\{d^2\left[rP(10;r)\right]/dr^2\right\}dr$$

Up to now, we have been using the symbol $P(n\ell;r)$ to denote the radial part of a single particle wave function. This is contrary to customary usage which ordinarily denotes by $P(n\ell;r)$ the radial wave function multiplied by r. We adopt this convention in the sequel, that is, $rP(n\ell;r)$. now stands for the function which in the foregoing notation would have been written $rP(n\ell; r)$.

From equations (2-28) and (2-29), we see that the expression

$$\int_0^\infty\left\{rP(10; r)\right\}\left\{d^2\left[rP(10; r)\right]/dr^2\right\}dr$$

occurs with a coefficient of $4! = 24$.

We note that part b) is a sum of integrals of the form

2-35 $$\int f_{P_2}{}^* f_{q_2}\, d\tau_2 \int f_{P_3}{}^* f_{q_3}\, d\tau_3 \int f_{P_4}{}^* f_{q_4}\, d\tau_4 \int f_{P_1}{}^* (8/r_1) f_{q_1}\, d\tau_1$$

each of which is zero unless $P_2 = q_2$; $P_3 = q_3$; and $P_4 = q_4$. Just as before, for a fixed value of $P_1 = q_1$, there are six distinct permutations of the remaining indicies which fit this criterion. Thus part b) gives rise to

2-36 $$6\left[\int f_1^*(1)(8/r_1)f_1(1)d\tau_1 + \int f_2^*(1)(8/r_1)f_2(1)d\tau_1 + \int f_3^*(1)(8/r_1)f_3(1)d\tau_1 + \int f_4^*(1)(8/r_1)f_4(1)d\tau_1\right]$$

We also find

2-37 $$\int f_1^*(1)\ (8/r_1)f_1(1)d\tau_1 =$$
$$\int f_1^*(2)\ (8/r_2)f_1(2)d\tau_2 =$$
$$\int f_1^*(3)\ (8/r_3)f_1(3)d\tau_3 =$$
$$\int f_1^*(4)\ (8/r_4)f_1(4)d\tau_4$$

[where we are using the new definition of the P functions]

Thus the integral $\int\left[P(10;r)\right]^2(8/r)dr$ occurs in the evaluation of $\int\psi^* H\psi\, d\tau$ with a coefficient of 24. Combining our two results, we find that the integral

2-38 $$\int_0^\infty P(10;r)\left[d^2/dr^2 + (8/r)\right]P(10;r)dr =$$
$$\int_0^\infty P(10;r)\left\{d^2\left[P(10;r)\right]/dr^2\right\}dr +$$
$$\int_0^\infty P(10;r)(8/r)P(10;r)dr$$

occurs with a coefficient of 24 in the evaluation of $\int\psi^* H\psi\, d\tau$

This fact suggests the introduction of a special symbol

2-39 $$I(10) =$$
$$(-1/2)\int_0^\infty P(10;\ r)\left[d^2/dr^2 + (8/r)\right]P(10;\ r)dr$$

where we have inserted a factor of $-1/2$ to match with the original equations. More generally, we introduce the symbol

2-40 $$I(n\ell) = (-1/2)\int_0^\infty P(n\ell;\ r)\left[d^2/dr^2 + (2N/r)\right]P(n\ell;\ r)dr$$

The functions f_2, f_3, and f_4 will effect the introduction of the quantities I(10), I(20), and I(20) respectively into the evaluation of $\int \psi^* H \psi\, d\tau$, each with a coefficient of 24. Note that f_1 and f_2 each give rise to the same factor I(10) while f_3 and f_4 each give rise to the factor I(20).

3. USE OF THE CENTRAL FIELD FUNCTIONS

We turn now to an evaluation of the parts c), d), and e) of statement (2-26) as well as those parts which arise from the three analogous terms in the expression $\int \psi^* H \psi\, d\tau$. The calculation depends upon our ability to expand the factor $1/r_{ij}$ in a series of products whose factors are powers of r_i, r_j, and $u = \cos\theta_{ij}$, where θ_{ij} is the angle between the radii vectors of electrons i and j from the origin, $i \neq j$. Using the familiar law of cosines, we find

3-1 $$1/r_{ij} = 1/\left[r_i^2 + r_j^2 - 2r_i r_j \cos\theta_{ij}\right]$$

The expression $\cos\theta_{ij}$ can be evaluated by means of the identity $\cos\theta_{ij} =$

$$\cos\theta_i \cos\theta_j + \sin\theta_i \sin\theta_j \cos(\Phi_i - \Phi_j)$$

where (r_i, θ_i, Φ_i) and (r_j, θ_j, Φ_j) are the spherical polar co-ordinates of electrons i and j, respectively.

We find it useful to introduce the function

3-2 $$U_k(r,s) = r^k/s^{k+1} \quad \text{for } r \leq s, \text{ and}$$
$$= s^k/r^{k+1} \quad \text{for } r \geq s.$$

Then it can be shown that $1/r_{ij}$ can be expanded in a series of Legendre polynomials of the form

3-3 $$1/r_{ij} = \sum_{k=0}^{\infty} U_k(r_i,r_j)P_k(\cos\theta_{ij}) = \sum_{k=0}^{\infty} U_k(r_i,r_j)P_k(u),$$

where $P_k(\cos\theta_{ij}) = P_k(u)$ is the Legendre polynomial of order k.

Before working with the particular problem at hand, let us look briefly at the much more general problem of evaluating the quantity which we shall denote by

3-4 $$(ab|q|cd) = \iint f^*_a(1)f^*_b(2)(1/r_{12})f_c(1)f_d(2)d\tau_1 d\tau_2$$

where, without loss of generality, we shall restrict our discussion to i=1, j=2. Here a, b, c, and d each specify a complete set of quantum numbers (n, ℓ, m, γ) while the integration is over both the co-ordinate and the spin spaces.

The part of this double integral independent of spin can be written, with the use of the expansion of $1/r_{12}$, in the form

3-5 $$\sum_{k=0}^{\infty}\Big\{\int_0^{\infty}\int_0^{\infty} U_k(r_1,r_2)P(n_a\ell_a;\, r_1)P(n_b\ell_b;\, r_2)P(n_c\ell_c;\, r_1)P(n_d\ell_d;\, r_2)dr_1dr_2$$
$$\int_0^{\pi}\int_0^{2\pi}\int_0^{\pi}\int_0^{2\pi} P_k(u)\theta_{\ell_a m_a}(\theta_1)\theta_{\ell_b m_b}(\theta_2)\theta_{\ell_c m_c}(\theta_1)\theta_{\ell_d m_d}(\theta_2)$$
$$\Phi^*_{m_a}(\Phi_1)\Phi^*_{m_b}(\Phi_2)\Phi_{m_c}(\Phi_1)\Phi_{m_d}(\Phi_2)\sin\theta_1\sin\theta_2 d\theta_1 d\Phi_1 d\theta_2 d\Phi_2\Big\}$$

where the $\Theta_{\ell m}(\Theta)$ and $\Phi_m(\Phi)$ denote the same functions of our earlier discussions. Fortunately, for our evaluation of these integrals, the Legendre polynomials are expandible in terms of these same $\theta_{\ell m}(\theta)$ and $\Phi_m(\Phi)$ according to

3-6
$$P_\ell(u) = \frac{4}{2\ell+1}\sum_{m=-\ell}^{\ell}\theta_{\ell m}(\theta_1)\theta_{\ell m}(\theta_2)\Phi_m(\Phi_1)\Phi_m(\Phi_2)$$

Hence, for the kth term in the sum over k, we may write

3-7
$$\left[4/(2k+1)\right]\times\sum_{m=-k}^{k}\left\{\int_0^{\pi}\theta_{km}(\theta_1)\theta_{\ell_a m_a}(\theta_1)\theta_{\ell_c m_c}(\theta_1)\sin\theta_1 d\theta_1 \int_0^{\pi}\Phi_m(\Phi_1)\Phi^*_{m_a}(\Phi_1)\Phi_{m_c}(\Phi_1)d\Phi_1 \int_0^{\pi}\theta_{km}(\theta_2)\theta_{\ell_b m_b}(\theta_2)\theta_{\ell_d m_d}(\theta_2)\sin\theta_2 d\theta_2 \int_0^{2\pi}\Phi_m(\Phi_2)\Phi^*_{m_b}(\Phi_2)\Phi_{m_d}(\Phi_2)d\Phi_2\right\}.$$

The Φ integrals, involving only exponentials, can be easily evaluated to give

$$(1/2\pi)\delta_{m,m_a-m_c}\delta_{m,m_d-m_b}.$$

Hence, in the summation over m, everything vanishes unless

$$m_a + m_b = m_c + m_d.$$

When this is true, as in our case, only the term remains where

3-8
$$m = m_a - m_c = m_d - m_b.$$

When this condition is satisfied, the angle factor reduces to

$$c^k(\ell_a m_a, \ell_c m_c)c^k(\ell_d m_d, \ell_b m_b),$$

where we have introduced the symbol

3-9 $$c^k(\ell m, \ell' m') = \sqrt{\frac{2}{2k+1}} \int_0^{\pi} \theta_{k,m-m'}(\theta)\theta_{\ell m}(\theta)\theta_{\ell' m'}(\theta)\sin\theta d\theta.$$

This integral can be shown to have the property

3-10 $$c^k(\ell m, \ell' m') = (-1)^{m-m'} c^k(\ell' m', \ell m).$$

If we now introduce the symbol

3-11 $$R^k(n_a\ell_a n_b\ell_b, n_c\ell_c n_d\ell_d) = \int_0^{\infty}\int_0^{\infty} U_k(r_4, r_2)P(n_a\ell_a; r_1)P(n_b\ell_b; r_2)P(n_c\ell_c; r_1)P(n_d\ell_d; r_2)dr_1 dr_2$$

then we may write

3-12 $$(ab|q|cd) = (\delta_{\gamma_a,\gamma_c}\delta_{\gamma_b,\gamma_d}\delta_{m_a+m_b,m_c+m_d}) \times \sum_{k=|m|}^{\infty} c^k(\ell_a m_a, \ell_c m_c)c^k(\ell_d m_d, \ell_b m_b)R^k(n_a\ell_a n_b\ell_b, n_c\ell_c n_d\ell_d).$$

where the range of k may equally well be written from 0 to ∞, since c^k can be shown to vanish identically for $k < |m|$.

The values of R^k depend on the initial choice of the central field and must be calculated independently for each different choice. But the c's are definite integrals of three associated Legendre polynomials and hence, by known methods, may be calculated once for all. Tables of their values through $\ell = 3$ appear in Condon and Shortley's book The Theory of Atomic Spectra, p. 178-179.

It is critical to note that an investigation of the behavior of the c's would show that in order for $c^k(\ell m, \ell' m')$ to be different from zero the following conditions must be satisfied.

3-13 $$k + \ell + \ell' = 2q \qquad (q \text{ an integer})$$

and

3-14 $$|\ell - \ell'| \leq k \leq \ell + \ell'.$$

Let us define the two special symbols

3-15 $$J_{ab} = \iint |f_a(i)|^2 (1/r_{ij}) |f_b(j)|^2 d\tau_i d\tau_j$$

3-16 $$K_{ab} = \iint f_a^*(i) f_b^*(j) (1/r_{ij}) f_b(i) f_a(j) d\tau_i d\tau_j$$

Thus we see, in the notation just defined, that

3-17 $$(ab|q|ab) = J_{ab}, \text{ and}$$

$$(ab|q|ba) = K_{ab}.$$

We can now write

3-18 $$J_{ab} = \sum_{k=0}^{\infty} a_k(\ell_a m_a, \ell_b m_b) F_k(n_a \ell_a, n_b \ell_b), \text{ and}$$

3-19 $$K_{ab} = \delta_{\gamma_a \gamma_b} \sum_{k=0}^{\infty} b_k(\ell_a m_a, \ell_b m_b) G_k(n_a \ell_a, n_b \ell_b)$$

where a_k and b_k are defined in terms of the c^k by

3-20 $$a_k(\ell_a m_a, \ell_b m_b) = c_k(\ell_a m_a, \ell_a m_a) c^k(\ell_b m_b, \ell_b m_b)$$

3-21 $$b_k(\ell_a m_a, \ell_b m_b) = \left[c^k(\ell_a m_a, \ell_b m_b)\right]^2$$

and F_k and G_k are special cases of R^k, namely

3-22 $$F_k(n_a \ell_a, n_b \ell_b) = R^k(n_a \ell_a n_b \ell_b, n_a \ell_a n_b \ell_b) = \int_0^\infty \int_0^\infty U_k(r_1, r_2) \left[P(n_a \ell_a; r_1)\right]^2 \left[P(n_b \ell_b; r_2)\right]^2 dr_1 dr_2$$

and

3-23 $$G_k(n_a \ell_a, n_b \ell_b) = R^k(n_a \ell_a n_b \ell_b, n_b \ell_b n_a \ell_a) = \int_0^\infty \int_0^\infty U_k(r_1, r_2) P(n_a \ell_a; r_1) P(n_b \ell_b; r_1) P(n_a \ell_a; r_2) P(n_b \ell_b; r_2) dr_1 dr_2 =$$

$$2 \int_0^\infty dr_2 \int_0^{r_2} \frac{r_1^k}{r_2^{k+1}} P(n_a \ell_a; r_1) P(n_b \ell_b; r_1) P(n_a \ell_a; r_2) P(n_b \ell_b; r_2) dr_1$$

Notice that even though the expressions (3-18) and (3-19) appear as infinite sums, there are only a finite number of non-zero terms because of the properties of c^k mentioned in preceeding discussion. In particular, for the case of beryllium, since $\ell = \ell' = 0$, the only non-zero summand is for $k = 0$. Furthermore, it should be pointed out that, because of the requirement that $k + \ell + \ell'$ be even in order that c^k be different from zero, in the expression for J_{ab} only those summands with even values for k give non-zero contributions. Consequently, the table of values of a_k has non-zero entries only for even k.

Let us return to the problem at hand, that is, to the particular case of beryllium corresponding to $(1s)^2(2s)^2$. Since $\ell = \ell' = m = m' = 0$, we have only summands different from zero in case $k = 0$ so that the only required value of the c's is

3-24 $$c^0(00,00) = \sqrt{2}/1 \int_0^{\pi} (\sqrt{2}/2)(\sqrt{2}/2)(\sqrt{2}/2)\sin\theta\, d\theta = 1/2 \int_0^{\pi} \sin\theta\, d\theta = 1.$$

Hence $a_o(00,00) = 1$ and $b_o(00,00) = 1$, which could have also been obtained from the tables mentioned earlier.

Consequently the contribution to E' from the J_{ab} and K_{ab} terms is simply

3-25
$$J(200+)(200-)+ J(200+)(100+)+ J(200+)(100-) +$$
$$J(200-)(100+)+ J(200-)(100-)+ J(100+)(100-) -$$
$$K(200+)(200-)- K(200+)(100+)- K(200+)(100-) -$$
$$K(200-)(100+)- K(200-)(100-)- K(100+)(100-) =$$
$$F_o(20,20) + F_o(20,10) + F_o(20,10) + F_o(20,10) +$$
$$F_o(20,10) + F_o(10,10) - 0 - G_o(20,10) -$$
$$0 - 0 - G_o(20,10) - 0 =$$

$$F_o(10,10) + F_o(20,20) + 4F_o(20,10) - 2G_o(20,10).$$

From the definitions of F_k and G_k, we see that for any fixed k, n, and ℓ

3-26
$$G_k(n\ell,n\ell) = F_k(n\ell,n\ell).$$

Furthermore if a and b are subscripts of a pair of distinct wave functions, then the coefficient a_o is always 1; and if we denote by $q(n\ell)$ the number of occupied wave function within a single group $(n\ell)$ there are $q(n\ell)\left[q(n\ell) - 1\right]/2$ such pairs. Consequently, the coefficient of each $F_o(n\ell,n\ell)$ is always $q(n\ell)\left[q(n\ell) - 1\right]/2$. Similarly, if $(n'\ell') \neq (n\ell)$, then the coefficient of each $F_o(n\ell,n'\ell')$ is $q(n\ell)q(n'\ell')$.

The a_k have the further property that for $k > 0$ and for a <u>complete</u> group

3-27
$$\sum_{m_b} a_k(\ell_a m_a, \ell_b m_b) = 0$$

for all m_a, the sum being over all values of m_b in the complete group $(n_b\ell_b)$. Hence, the only contributions to E' involving F_k integrals with $k > 0$ are of the form $F_k(n\ell,n\ell)$, since we can write

3-28
$$\sum_{a,b} J_{ab} = \sum_{(n\ell m\gamma)(n'\ell'\gamma')} \sum_{k=0}^{\ell+\ell'} a_k(\ell m,\ell' m') F_k(n\ell,n'\ell') =$$

$$\sum_{k=0}^{\ell+\ell'} \sum_{(n\ell\gamma)(n'1'\gamma')} F_k(n\ell,n'\ell') \sum_{m,m'} a_k(\ell m,\ell' m')$$

This result is not needed in the case of beryllium since we never have $k > 0$.

For a configuration of complete groups, E' is reduced to a sum of multiples of $I(n\ell)$, $F_o(n\ell,n'\ell')$, $F_k(n\ell,n\ell)$, and $G_k(n\ell,n'\ell')$ such as

3-29
$$E' =$$

$$\sum_n q(n\ell) I(n\ell) + \sum_{n\ell} (1/2) q(n\ell)\left[q(n\ell)-1\right] F_o(n\ell,n\ell) +$$

$$\sum_{n\ell,n'\ell'\neq n} q(n\ell) q(n'\ell\ell) F(n\ell,n'\ell') -$$

$$\sum_{n\ell k} A_{\ell k} F_k(n\ell,n\ell) - \sum_{n\ell,n'\ell',k} B_{\ell\ell' k} G_k(n\ell,n'\ell') .$$

where the last two contributions were written with negative signs so that the values of the coefficients $A_{\ell k}$ and $B_{\ell\ell' k}$ are positive. The values of these coefficients can be calculated from the tables of values of the a_k and b_k . They are tabulated in Hartree's book The Calculation of Atomic Structures, p. 50.

For the case of beryllium $(1s)^2(2s)^2$, we see that this formula yields

3-30
$$E' =$$

$$2I(10) + 2I(20) + F_o(10,10) +$$

$$F_o(20,20) + 4F_o(20,10) - 2G_o(20,10)$$

which is in complete agreement with our previous results.

If we return to the previously introduced notation and look at the case for beryllium, then

3-31 $$\psi = \sum_{P\epsilon S_4} \delta_P P\left[f_1(1)f_2(2)f_3(3)f_4(4)\right]$$

$$\psi^* = \sum_{P\epsilon S_4} \delta_P P\left[f_1^*(1)f_2^*(2)f_3^*(3)f_4^*(4)\right]$$

and, as we have seen, the evaluation of $\int \psi^* H \psi \, d\tau$ has terms involving $\frac{1}{r_{ij}}$. If, for example, we consider that term which involves $\frac{1}{r_{12}}$ then we get

3-32 $$\int\left[\sum_{P\epsilon S_4} \delta_P P\left\{f_1^*(1)f_2^*(2)f_3^*(3)f_4^*(4)\right\}\right]\left[\frac{1}{r_{12}}\right] \times$$
$$\times\left[\sum_{Q\epsilon S_4} \delta_Q Q\left\{f_1(1)f_2(2)f_3(3)f_4(4)\right\}\right]d\tau =$$
$$\sum_{PQ}\sum \delta_P\delta_Q P\left\{f_1^*(1)f_2^*(2)f_3^*(3)f_4^*(4)\right\}\left(\frac{1}{r_{12}}\right)\times$$
$$\times Q\left\{f_1(1)f_2(2)f_3(3)f_4(4)\right\}d\tau\Big] =$$
$$\sum_{PQ}\sum \delta_P\delta_Q \int f_{p_1}^*(1)f_{p_2}^*(2)f_{p_3}^*(3)f_{p_4}^*(4)\frac{1}{r_{12}} \times$$
$$\times f_{q_1}(1)f_{q_2}(2)f_{q_3}(3)f_{q_4}(4)d\tau_1 d\tau_2 d\tau_3 d\tau_4 =$$
$$\sum_{PQ}\sum \delta_P\delta_Q \int f_{p_3}^*(3)f_{q_3}(3)d\tau_3 \int f_{p_4}^*(4)f_{q_4}(4)d\tau_4 \times$$
$$\times\iint f_{p_1}^*(1)f_{q_1}(1)\frac{1}{r_{12}}f_{p_2}^*(2)f_{q_2}(2)d\tau_1 d\tau_2\Big]$$

Clearly this term is zero unless $p_3 = q_3$ and $p_4 = q_4$, so that this term is zero unless 1) $p_1 = q_1$ and $p_2 = q_2$ or 2) $p_1 = q_2$ and $p_2 = q_1$.

For each choice of $p_1 = q_1$ and $p_2 = q_2$ there are 2 choices for $p_3 = q_3$, after which $p_4 = q_4$ is determined, that is, there are 2 distinct permutations of the remaining indices which satisfy the criteria. Furthermore, in this case, P = Q so that $\delta_P = \delta_Q$ and $\delta_P\delta_Q = 1$.

Similarly, for each choice of $p_1 = q_2$ and $p_2 = q_1$ there are 2 distinct permutations of the remaining indices. However, in this case, P and Q differ by a transposition so that $\delta_P = -\delta_Q$ and $\delta_P\delta_Q = -1$.

Hence we see that for the case when $p_1 = q_1$ and $p_2 = q_2$ we get integrals of the form

3-33 $$2\iint f_{p_1}^*(1)f_{p_1}(1)\frac{1}{r_{12}}f_{p_2}^*(2)f_{p_2}(2)d\tau_1 d\tau_2$$

$$=\iint |f_{p_1}(1)|^2\frac{1}{r_{12}}|f_{p_2}(2)|^2 d\tau_1 d\tau_2$$

which corresponds, in form, to a $J_{p_1p_2}$ type integral. But in the case when $p_1 = q_2$ and $p_2 = q_1$ we get integrals of the form

3-34 $$-2\iint f_{p_1}^*(1)f_{p_2}(1)\frac{1}{r_{12}}f_{p_2}^*(2)f_{p_1}(2)d\tau_1 d\tau_2$$

which corresponds, in form, to a $K_{p_1p_2}$ type integral.

Furthermore we can see that these terms are the same for each choice of the variables of integration, i.e.

3-35 $$\iint f_{p_1}^*(1)f_{q_1}(1)\frac{1}{r_{12}}f_{p_2}^*(2)f_{q_2}(2)d\tau_1 d\tau_2$$

$$=\iint f_{p_1}^*(1)f_{q_1}(1)\frac{1}{r_{13}}f_{p_2}^*(3)f_{q_2}(3)d\tau_1 d\tau_3$$

$$= \cdots\cdots$$

and there are $\frac{(4)(3)}{2}$ ways of choosing the variables of integration, so that these integrals appear with coefficients of $\frac{4!}{2} = 12$.

4. THE Y_k AND Z_k FUNCTIONS

We wish to derive the differential equation whose solution is the radial wave function P(n0; r). Let

4-1 $$Y_o(n0,n'0;\ r) = r\int_o^\infty U_o(r,s)P(n0;\ s)P(n'0;\ s)ds$$

where

4-2 $$U_o(r,s) = 1/s \text{ when } r \leq s, \text{ and}$$
$$= 1/r \text{ when } r > s.$$

4-3 $$Y_o(n0,n'0;\ r) = r\int_0^r U_o(r,s)P(n0;\ s)P(n'0;\ s)ds + r\int_r^\infty U_o(r,s)P(n0;\ s)P(n'0;\ s)ds =$$
$$\int_o P(n0;\ s)P(n'0;\ s)ds + \int_r^\infty (r/s)P(n0;\ s)P(n'0;\ s)ds$$

Define the functions

4-4 $$F_o(n0,n'0) = \int_o^\infty\int_o^\infty P^2(n0;\ r)P^2(n'0;\ s)U_o(r,s)drds =$$
$$\int_o^\infty P^2(n0;\ r)(1/r)Y_o(n'0,n'0;\ r)dr =$$
$$\int_o^\infty P^2(n'0;\ r)(1/r)Y_o(n0,n0;\ r)dr$$

and

4-5 $$G_o(n0,n'0) = \int_o^\infty\int_o^\infty P(n0;\, r)P(n'0;\, r)U_o(r,s)P(n0;\, s)P(n'0;\, s)drds = \int_o^\infty P(n0;\, r)P(n'0;\, r)(1/r)Y_o(n0,n'0;\, r)dr$$

Now let

4-6 $$Z_o(n0,n'0;\, r) = \int_o^r P(n0;\, s)P(n'0;\, s)ds, \quad r \geq 0$$

Differentiating with respect to r, we obtain the differential equation.

4-7 $$d\left[Z_o(n0,n'0;\, r)\right]/dr = P(n0;\, r)P(n'0;\, r)$$

Substituting $Z_o(n0,n'0;r)$ for the first integral of $Y_o(n0,n'0;\, r)$, we get

$$Y_o(n0,n'0;\, r) = Z_o(n0,n'0;\, r) + \int_r^\infty (r/s)P(n0;\, s)P(n'0;\, s)\, ds$$

Multiplying by r^{-1} we get

$$r^{-1}Y_o(n0,n'0;\, r) = r^{-1}Z_o(n0,n'0;\, r) + \int_r^\infty \left(\frac{1}{s}\right)P(n0;\, s)P(n'0;\, s)ds$$

Differentiating with respect to r, we get

$$-r^{-2}Y_o(n0,n'0;\, r) + r^{-1}\frac{dY_o}{dr}(n0,n'0;\, r) = -r^{-2}Z_o(n0,n'0;\, r) + r^{-1}\frac{dZ_o}{dr}(n0,n'0;\, r) - \frac{1}{r}P(n0;\, r)P(n'0;\, r)$$

Substituting our expression for $\frac{dZ_o}{dr}(n0,n'0;\, r)$, we obtain

$$\frac{-1}{r}Y_o(n0,n'0;\, r) + \frac{dY_o}{dr}(n0,n'0;\, r) = \frac{-1}{r}Z_o(n0,n'0;\, r) + P(n0;\, r)P(n'0;\, r) - P(n0;\, r)P(n'0;\, r)$$

4-8 $$\frac{dY_o}{dr}(n0,n'0;\, r) = -\frac{1}{r}\left[Z_o(n0,n'0;\, r) - Y_o(n0,n'0;\, r)\right]$$

Now $$Y_o(n0,n'0;\, r) - Z_o(n0,n'0;\, r) = \int_r^\infty \left(\frac{r}{s}\right)P(n0;\, s)P(n'0;\, s)ds$$

4-9 $$\lim_{r\to\infty}\left[Y_o(n0,n'0;\ r) - Z_o(n0,n'0;\ r)\right] = \lim_{r\to\infty}\int_r^\infty \left(\frac{r}{s}\right)P(n0;\ s)P(n'0;\ s)ds$$

$= 0$ by the nature of the radial function $P(n0;\ r)$.

Differentiating equation (4-8) with respect to r we get

$$\frac{d^2Y_o}{dr^2}(n0,n'0;\ r) = \frac{1}{r^2}\left[Z_o(n0,n'0;\ r) - Y_o(n0,n'0;\ r)\right] -$$

$$\frac{1}{r}\left[\frac{dZ_o}{dr}(n0,n'0;\ r) - \frac{dY_o}{dr}(n0,n'0;\ r)\right] =$$

$$\frac{1}{r^2}\left[Y_o(n0,n'0;\ r) - r\,\frac{dY_o}{dr}(n0,n'0;\ r) - Y_o(n0,n'0;\ r)\right] -$$

$$\frac{1}{r}\left[P(n0;\ r)P(n'0;\ r) - \frac{dY_o}{dr}(n0,n'0;\ r)\right]$$

Hence we have the differential equation

4-10 $$\frac{d^2Y_o}{dr^2}(n0,n'0;\ r) + \frac{1}{r}P(n0;\ r)P(n'0;\ r) = 0$$

LEMMA: Let $u(x)$ and $v(x)$ have second derivatives and $u(a) = v(a) = u(b) = v(b) = 0$. Then

4-11 $$\int_a^b u\frac{d^2v}{dx}dx = \int_a^b v\frac{d^2u}{dx^2}dx.$$

Proof: $$\frac{d}{dx}\left(\frac{udv}{dx} - \frac{vdu}{dx}\right) = \frac{ud^2v}{dx^2} + \frac{du}{dx}\frac{dv}{dx} - \frac{vd^2u}{dx^2} - \frac{dv}{dx}\frac{du}{dx}$$

$$\int_a^b d\left(\frac{udv}{dx} - \frac{vdu}{dx}\right) = \int_a^b \frac{ud^2v}{dx^2}\,dx - \int_a^b \frac{vd^2u}{dx^2}\,dx$$

$$\int_a^b d\left(\frac{udv}{dx} - \frac{vdu}{dx}\right) = \frac{udv}{dx} - \frac{vdu}{dx}\Big|_a^b = 0.$$

Thus $$\int_a^b \frac{ud^2v}{dx^2}dx = \int_a^b \frac{vd^2u}{dx^2}dx.$$

We have shown (where I, F, and G denote the new functions) that

4-12 $$E' = 2I(10) + 2I(20) + F_o(10,10) +$$

$$4F_o(10,20) + F_o(20,20) - 2G_o(10,20)$$

We select the radial functions $P(10;\ r)$ and $P(20;\ r)$ so as to

minimize the value of E' and such that

4-13 $$P(1s; 0) = P(2s; 0) = \lim_{r\to\infty} P(1s; r) = \lim_{r\to\infty} P(2s; r) = 0$$

We want to construct a function $E'(\epsilon_{1s},\epsilon_{2s})$ such that

4-14 $$E'(0,0) = E'$$

To construct this function, let

4-15 $$\bar{P}(1s; r) = P(1s; r) + \epsilon_{1s}\Delta P(1s; r) \text{ and}$$

$$\bar{P}(2s; r) = P(2s; r) + \epsilon_{2s}\Delta P(2s; r), \text{ where}$$

$$\Delta P(1s; 0) = \Delta P(2s; 0) = \lim_{r\to\infty} \Delta P(1s; r) = \lim_{r\to\infty} \Delta P(2s; r) = 0$$

and define the functions

4-16 $$I(1s,\epsilon_{1s}) = -\frac{1}{2}\int_0^\infty \bar{P}(1s; r)\left[\frac{d^2}{dr^2} + \frac{8}{r}\right]\bar{P}(1s; r)dr$$

$$F_o(1s,1s,\epsilon_{1s}) =$$
$$\int_0^\infty \bar{P}(1s; r)(1/r)\left\{\int_0^r \bar{P}^2(1s; s)ds + \int_r^\infty (r/s)\bar{P}^2(1s; s)ds\right\}dr$$

$$F_o(1s,2s,\epsilon_{1s},\epsilon_{2s}) =$$
$$\int_0^\infty\int_0^\infty \bar{P}^2(1s; r)U_o(r,s)\bar{P}^2(2s; r)dr$$

$$G_o(1s,2s,\epsilon_{1s},\epsilon_{2s}) =$$
$$\int_0^\infty \bar{P}(1s; r)\bar{P}(2s; r)(1/r)\left\{\int_0^r \bar{P}(1s; s)\bar{P}(2s; s)ds + \right.$$
$$\left.\int_r^\infty (r/s)\bar{P}(1s; s)\bar{P}(2s; s)ds\right\}dr$$

$I_o(2s,\epsilon_{2s})$ and $F_o(2s,2s,\epsilon_{2s})$ are defined in a similar fashion. The desired function is:

4-17 $$E'(\epsilon_{10},\epsilon_{20}) =$$

$$2I(10,\epsilon_{10}) + 2I(20,\epsilon_{20}) +$$

$$F_o(10,10,\epsilon_{10}) + F_o(20,20,\epsilon_{20}) +$$

$$4F_o(10,20,\epsilon_{10},\epsilon_{20}) - 2G_o(10,20,\epsilon_{10},\epsilon_{20})$$

Since P(10; r) and P(20; r) were chosen so as to minimize E', both $\frac{\partial E'}{\partial \epsilon_{10}}(0,0)$ and $\frac{\partial E'}{\partial \epsilon_{20}}(0,0)$ will be zero.

We wish to carry out these partial derivatives in detail.

4-18 $$\frac{\partial E'}{\partial \epsilon_{10}}(\epsilon_{10},\epsilon_{20}) = \frac{2\partial I}{\partial \epsilon_{10}}(10,\epsilon_{10}) + \frac{\partial F_o}{\partial \epsilon_{10}}(10,10,\epsilon_{10}) +$$

$$\frac{4\partial F_o}{\partial \epsilon_{10}}(10,20,\epsilon_{10},\epsilon_{20}) - \frac{2\partial G_o}{\partial E_{10}}(10,20,\epsilon_{10},\epsilon_{20})$$

4-19 $$\frac{\partial E'}{\partial \epsilon_{20}}(\epsilon_{10},\epsilon_{20}) =$$

$$\frac{2\partial I}{\partial \epsilon_{20}}(20,\epsilon_{20}) + \frac{4\partial F_o}{\partial \epsilon_{20}}(10,20,\epsilon_{10},\epsilon_{20}) + \frac{\partial F_o}{\partial \epsilon_{20}}(20,20,\epsilon_{20}) -$$

$$\frac{2\partial G_o}{\partial \epsilon_{20}}(10,20,\epsilon_{10},\epsilon_{20}) .$$

We will evaluate two of these components separately. The others are evaluated in like manner and only the results will be stated.

$$I(10,\epsilon_{10}) = -\frac{1}{2}\int_o^\infty (P+\epsilon_{10}\Delta P)(10; r)\left[\frac{d^2}{dr^2} + \frac{8}{r}\right](P+\epsilon_{10}\Delta P)(10; r)dr$$

4-20 $$\frac{\partial I}{\partial \epsilon_{10}}(10,\epsilon_{10}) = -\frac{1}{2}\int_o^\infty (P+\epsilon_{10}\Delta P)(10; r)\left[\frac{d^2}{dr^2} + \frac{8}{r}\right]\Delta P(10; r)dr -$$

$$\frac{1}{2}\int_o^\infty \Delta P(10; r)\left[\frac{d^2}{dr^2} + \frac{8}{r}\right](P+\epsilon_{10}\Delta P)(10; r)dr.$$

$$\frac{\partial I}{\partial \epsilon_{10}}(10,0) = -\frac{1}{2}\int_o^\infty P(10; r)\left[\frac{d^2}{dr^2} + \frac{8}{r}\right]\Delta P(10; r)dr -$$

$$\frac{1}{2}\int_o^\infty \Delta P(10; r)\left[\frac{d^2}{dr^2} + \frac{8}{r}\right]P(10; r)dr =$$

$$-\int_o^\infty \Delta P(10;\ r)\ \frac{d^2}{dr^2} + \frac{8}{r}\ P(10;\ r)dr. \quad \text{(by the Lemma).}$$

$$F_o(10,10,\epsilon_{10}) = \int_o^\infty (P+\epsilon_{10}\Delta P)^2(10;\ r)\underline{1}_r\Big\{\int_o^r (P+\epsilon_{10}\Delta P)^2(10;\ s)ds +$$

$$\int_r^\infty (r/s)(P+\epsilon_{10}\Delta P)^2(10;\ s)ds\Big\}dr =$$

$$\int_o^\infty \Big[P^2+2\epsilon_{10}P\Delta P+\epsilon_{10}{}^2(\Delta P)^2\Big](10;\ r)\ \times$$

$$1/r\Big\{\int_o^r \Big[P^2+2\epsilon_{10}P\Delta P+\epsilon_{10}{}^2(\Delta P)^2\Big](10;\ s)ds +$$

$$\int_r^\infty (r/s)\Big[P^2+2\epsilon_{10}P\Delta P+\epsilon_{10}{}^2(\Delta P)^2\Big](10;\ s)ds\Big\}dr$$

4-22 $$\frac{\partial F_o}{\partial \epsilon_{10}}(10,10,\epsilon_{10}) = \int_o^\infty \Big[2P\Delta P+2\epsilon_{10}(\Delta P)^2\Big](10;\ r)\ \times$$

$$1/r\Big\{\int_o^r \Big[P^2+2\epsilon_{10}P\Delta P+\epsilon_{10}{}^2(\Delta P)^2\Big](10;\ s)ds +$$

$$\int_r^\infty (r/s)\Big[P^2+2\epsilon_{10}P\Delta P+\epsilon_{10}{}^2(\Delta P)^2\Big](10;\ s)ds\Big\}dr +$$

$$\int_o^\infty \Big[P^2+2\epsilon_{10}P\Delta P+\epsilon_{10}{}^2(\Delta P)^2\Big](10;\ r)\ \times$$

$$1/r\Big\{\int_o^r \Big[2P\Delta P+2\epsilon_{10}(\Delta P)^2\Big](10;\ s)ds +$$

$$\int_r^\infty (r/s)\Big[2P\Delta P+2\epsilon_{10}(\Delta P)^2\Big](10;\ s)ds\Big\}dr$$

4-23 $$\frac{\partial F_o}{\partial \epsilon_{10}}(10,10,0) = \int_o^\infty 2P\Delta P(10;\ r)\underline{1}_r Y_o(10,10;\ r)dr +$$

$$\int_o^\infty P(10;\ r)\underline{1}_r\Big\{\int_o^r 2P\Delta P(10;\ s)ds + \int_r^\infty (r/s)2P\Delta P\Big](10;\ s)ds\Big\}dr =$$

$$\int_o^\infty \Delta\Big[P^2(10;\ r)\Big]\underline{1}_r Y_o(10,10;\ r)dr +$$

$$\int_0^\infty P^2(10;\, r)\frac{1}{r}\left\{\int_0^r\left[P^2(10;\, s)\right]ds + \int_r^\infty\left(\frac{r}{s}\right)\left[P^2(10;\, s)\right]ds\right\}dr =$$

$$\int_0^\infty \Delta\left[P^2(10;\, r)\right]\frac{1}{r}Y_0(10,10,r)dr + \int_0^\infty P^2(10;\, r)\frac{1}{r}\Delta Y_0(10,10;\, r)dr =$$

$$\int_0^\infty \Delta\left[P^2(10;\, r)\right]\frac{1}{r}Y_0(10,10;\, r)dr + \int_0^\infty \Delta\left[P^2(10;\, r)\right]\frac{1}{r}Y_0(10,10;\, r)dr =$$

$$4\int_0^\infty P(10;\, r)\Delta P(10;\, r)\frac{1}{r}Y_0(10,10;\, r)dr.$$

4-24 $$\frac{\partial F_o}{\partial \epsilon_{10}}(10,20,0,0) = 2\int_o^\infty P(10;\ r)\Delta P(10;\ r)(1/r)Y_o(20,20;\ r)dr$$

4-25 $$\frac{\partial G_o}{\partial \epsilon_{10}}(10,20,0,0) = 2\int_o^\infty P(20;\ r)\Delta P(10;\ r)(1/r)Y_o(10,20;\ r)dr$$

For the other partial derivatives replace 10 by 20 and 20 by 10.

By observing that each term in the integrand of the first equation has the factor $\Delta P(10;\ r)$, we can write $\partial E'(0,0)/\partial \epsilon_{10}$ in the form

4-26 $$\int_o^\infty \Delta P(10;\ r)Q(10;\ r)dr$$

where $Q(10;\ r)$ is the sum of the remaining factors multiplied by their corresponding coefficients. Similarly, $\partial E'(0,0)/\partial \epsilon_{20}$ can be written in the form

4-27 $$\int_o^\infty \Delta P(20;\ r)Q(20;\ r)dr$$

By the above process we can show that at $\epsilon_{10} = \epsilon_{20} = 0$

4-28 $$\partial\left[\int_o^\infty \bar{P}^2(10;\ r)dr\right]/\partial \epsilon_{10} = 2\int_o^\infty \Delta P(10;\ r)P(10;\ r)dr$$

4-29 $$\partial\left[\int_o^\infty \bar{P}(10;\ r)\bar{P}(20;\ r)dr\right]/\partial \epsilon_{10} = \int_o^\infty \Delta P(10;\ r)P(20;\ r)dr$$

We obtain two similar expressions by evaluating derivatives with respect to ϵ_{20} at ϵ_{10} and ϵ_{20} equal to zero.

We wish to minimize $E'(\epsilon_{10},\epsilon_{20})$ subject to the additional conditions

4-30 $$\int_o^\infty P(n0;\ r)P(n'0;\ r)dr = \delta_{nn'}$$

We use the method of Lagrange multipliers which are denoted by $\epsilon_{10,10}$, $\epsilon_{10,20}$, $\epsilon_{20,10}$, and $\epsilon_{20,20}$. We obtain variational equations of the form

4-31
$$\int_0^\infty \Delta P(10;\, r)Q(10;\, r)dr \;+\; 2\epsilon_{10,10}\int_0^\infty \Delta P(10;\, r)P(10;\, r)dr \;+\; 2\epsilon_{10,20}\int_0^\infty \Delta P(10;\, r)P(20;\, r)dr \;=\; 0$$

which may be rewritten

$$\int_0^\infty \Delta P(10;\, r)\Big[Q(10;\, r) + 2\epsilon_{10,10}P(10;\, r) + 2\epsilon_{10,20}P(20;\, r)\Big]dr \;=\; 0$$

from which it follows that

4-32
$$Q(10;\, r) + 2\Big[\epsilon_{10,10}P(10;\, r) + \epsilon_{10,20}P(20;\, r)\Big] \;=\; 0$$

In a similar manner, we find

4-33
$$Q(20;\, r) + 2\Big[\epsilon_{20,20}P(20;\, r) + \epsilon_{20,10}P(10;\, r)\Big] \;=\; 0$$

These equations (4-32 and 4-33) are the Hartree-Fock equations in a non-standard form.

5. THE HARTREE-FOCK EQUATIONS OF NORMAL BERYLLIUM

The normal configuration of beryllium has two electrons in a 1s state and two electrons in a 2s state. Consequently there are two Hartree-Fock equations for the two "so-called" radial wave-functions, P(10; r) and P(20; r). One notes, of course, that P(10; r) and P(20; r) differ by a factor of r from the actual wave-functions.

We recall that the variation of E' is

5-1 $$\Delta E' = \int_0^\infty \Delta P(n\ell; r)Q(n\ell; r)dr$$

due to a variation $\Delta P(n\ell; r)$ of the wave-function $P(n\ell; r)$.

The various contributions to Q(10; r) are

5-2 $$\Delta I(10) = -2\left[d^2/dr^2 + 8/r\right]P(10; r)$$

$$\Delta F_o(10,10) = (4/r)Y_o(10,10; r)P(10; r)$$

$$\Delta F_o(10,20) = (8/r)Y_o(20,20; r)P(10; r)$$

$$\Delta G_o(10,20) = -(4/r)Y_o(10,20; r)P(20; r).$$

There is a further contribution from the Lagrange multipliers of the form

5-3 $$2\left\{\epsilon_{10,10}P(10; r) + \epsilon_{10,20}P(20; r)\right\}.$$

The final result after applying calculus of variation techniques to obtain the Euler-Lagrange equation for P(10; r) is

5-4 $$-2\left[d^2/dr^2 + 8/r\right]P(10; r) +$$

$$(4/r)Y_o(10,10; r)P(10; r) +$$

$$(8/r)Y_o(20,20; r)P(10; r) =$$

$$(4/r)Y_o(10,20; r)P(20; r) +$$

$$2\epsilon_{10,10}P(10; r) + 2\epsilon_{10,20}P(20; r) = 0$$

Upon factoring out -2 and rearranging some terms, we obtain the equation

5-5 $$\left\{d^2/dr^2 + 8/r - (2/r)Y_o(10,10; r) -\right.$$

$$\left.(4/r)Y_o(20,20; r) - \epsilon_{10,10}\right\}P(10; r) =$$

$$-(2/r)Y_o(10,20; r)P(20; r) + \epsilon_{10,20}P(20; r)$$

which may be rearranged to give the equation

5-6
$$\left\{d^2/dr^2 + (2/r)\left[4 - Y_o(10,10;\ r) - 2Y_o(20,20;\ r)\right] - \epsilon_{10,10}\right\}P(10;\ r) = -(2/r)Y_o(10,20;\ r)P(20;\ r) + \epsilon_{10,20}P(20;\ r)$$

We now choose to write the result in the form

5-7
$$\left\{d^2/dr^2 + (2/r)Y(10;\ r) - \epsilon_{10,10}\right\}P(10;\ r) = X(10;\ r) + \epsilon_{10,20}P(20;\ r)$$

where the various functions are defined by

$$Y(r) = 4 - 2Y_o(10,10;\ r) - 2Y_o(20,20;\ r)$$

$$Y(10;\ r) = Y(r) + Y_o(10,10;\ r)$$

$$X(10;\ r) = -(2/r)Y_o(10,20;\ r)P(20;\ r)$$

The various contributions for $n\ell = 20$ are

5-8
$$\Delta I(20) = -2\left[d^2/dr^2 + 8/r\right]P(20;\ r)$$

$$\Delta F_o(20,20) = (4/r)Y_o(20,20;\ r)P(20;\ r)$$

$$\Delta F_o(10,20) = (8/r)Y_o(10,10;\ r)P(20;\ r)$$

$$\Delta G_o(20,10) = -(4/r)Y_o(20,10;\ r)P(10;\ r)$$

The contribution from the Lagrange multipliers is

5-9
$$2\left\{\epsilon_{20,10}P(10;\ r) + \epsilon_{20,20}P(20;\ r)\right\}$$

Altogether we have the result

5-10
$$-2\left[d^2/dr^2 + 8/r\right]P(20;\ r) + (4/r)Y_o(20,20;\ r)P(20;\ r) + (8/r)Y_o(10,10;\ r)P(20;\ r) - (4/r)Y_o(20,10;\ r)P(10;\ r) + 2\left\{\epsilon_{20,10}P(10;\ r) + \epsilon_{20,20}P(20;\ r)\right\} = 0$$

After suitable rearrangements, we obtain

5-11 $$\left\{d^2/dr^2 + (2/r)Y(20;\ r) - \epsilon_{20,20}\right\}P(20;\ r) = X(20;\ r) + \epsilon_{20,10}P(10;\ r)$$

where

$$Y(r) = 4 - 2Y_o(10,10;\ r) - 2Y_o(20,20;\ r)$$

$$Y(20;\ r) = Y(r) + Y_o(20,20;\ r)$$

$$X(20;\ r) = -(2/r)Y_o(20,10;\ r)P(10;\ r)$$

In summary, we get two equations

5-12 $$\left\{d^2/dr^2 + (2/r)Y(10;\ r) - \epsilon_{10,10}\right\}P(10;\ r) = X(10;\ r) + \epsilon_{10,20}P(20;\ r)$$

5-13 $$\left\{d^2/dr^2 + (2/r)Y(20;\ r) - \epsilon_{20,20}\right\}P(20;\ r) = X(20;\ r) + \epsilon_{20,10}P(10;\ r)$$

Equations (5-12) and (5-13) are the Hartree-Fock equations <u>with exchange</u>.

6. <u>EQUATIONS WITHOUT EXCHANGE</u>

Consider the first Hartree-Fock equation in terms of $Y_o(n0,n'0;\ r)$,

6-1 $$\left[\frac{d^2}{dr^2} + \frac{2}{r}\left\{4 - Y_o(10,10;\ r) - 2Y_o(20,20;\ r)\right\} - \epsilon_{10,10}\right]P(10;\ r) = -\frac{2}{r}Y_o(10,20;\ r)P(20;\ r) + \epsilon_{10,20}P(20;\ r).$$

If we neglect the factors $Y_o(n0,n'0;\ r)$, $n0 \neq n'0$ and $\epsilon_{n0,n'0}$, $n0 \neq n'0$ we obtain zero on the right hand side of the equation. In the condensed notation we can then write

6-2 $$\left[\frac{d^2}{dr^2} + \frac{2}{r}Y(10;\ r) - \epsilon_{10,10}\right]P(10;\ r) = 0,$$

and similarly the second Hartree-Fock equation becomes

6-3 $$\left[\frac{d^2}{dr^2} + \frac{2Y(20;\ r)}{r} - \epsilon_{20,20}\right] P(20;\ r) = 0.$$

These are the Hartree-Fock equations without exchange.

We now wish to derive a differential equation relating Y(r) and Z(r) where

6-4 $$Y(r) = 4 - 2Y_o(10,10;\ r) - 2Y_o(20,20;\ r) \text{ and}$$

6-5 $$Z(r) = 4 - 2Z_o(10,10;\ r) - 2Z_o(20,20;\ r).$$

We know that

6-6 $$\frac{d}{dr} Y_o(n0,n0;\ r) = \frac{1}{r}\left[Y_o(n0,n0;\ r) - Z_o(n0,n0;\ r)\right].$$

Now,

6-7 $$\frac{d}{dr} Y(r) = \frac{d}{dr}\left[4 - 2Y_o(10,10;\ r) - 2Y_o(20,20;\ r)\right] =$$
$$-\frac{2}{r}\left[\left\{Y_o(10,10;\ r) - Z_o(10,10;\ r)\right\} +\right.$$
$$\left.\left\{Y_o(20,20;\ r) - Z_o(20,20;\ r)\right\}\right] =$$
$$\frac{1}{r}\left[4 - 2Y_o(10,10;\ r) - 2Y_o(20,20;\ r) -\right.$$
$$\left.\left\{4 - 2Z_o(10,10;\ r) - 2Z_o(20,20;\ r)\right\}\right].$$

Hence,

6-8 $$\frac{dY(r)}{dr} = \frac{1}{r}\left[Y(r) - Z(r)\right].$$

Assume the radial functions P(n0; r) to have the following two properties:

1. $P(n0;\ 0) = 0.$

2. P(n0; r) has a Taylor series expansion.

Let $P(10; r) = a_o + a_1 r + a_2 r^2 + \ldots$

and $P(20; r) = b_o + b_1 r + b_2 r^2 + \ldots.$

Since $P(10; 0) = P(20; 0) = 0$, $a_o = b_o = 0$.

Hence

6-9 $P(10; r) = a_1 r + a_2 r^2 + \ldots$

$P^2(10; r) = (a_1 r + a_2 r^2 + \ldots)(a_1 r + a_2 r^2 + \ldots) = a_1^2 r^2 + 2a_1 a_2 r^3 + \ldots.$

Now,

6-10 $$Z_o(10,10; r) = \int_o^r P^2(10; s)ds = \int_o^r (a_1 s^2 + 2a_1 a_2 s^3 + \ldots)ds =$$

$$\frac{a_1^2 s^3}{3} + 2a_1 a_2 \frac{s^4}{4} + \ldots \Big|_o^r =$$

$$\alpha_3 r^3 + \alpha_4 r^4 + \ldots =$$

$O(r^3)$, for small values of r.

Similarly,

6-11 $$Z_o(20,20; r) = \beta_3 r^3 + \beta_4 r^4 + \ldots.$$

Now,

6-12 $$\frac{4 - Z(r)}{r^2} = \frac{1}{r^2}\left[2Z_o(10,10; r) + 2Z_o(20,20; r)\right] =$$

$$\frac{1}{r^2}\left[2\alpha_3 r^3 + 2\alpha_4 r^4 + \ldots + 2\beta_3 r^3 + 2\beta_4 r^4 + \ldots\right] =$$

$$2(\alpha_3 + \beta_3) r + 2(\alpha_4 + \beta_4) r^2 + \ldots =$$

$O(r)$, for small values of r.

Now,

6-13 $$Y(r) = 4 - 2Y_o(10,10;\, r) - 2Y_o(20,20;\, r) =$$
$$4 - 2\left[\int_o^r P^2(10;\, s)ds + r\int_r^\infty \frac{P^2(10;\, s)}{s}ds\right] -$$
$$2\left[\int_o^r P^2(20;\, s)ds + r\int_r^\infty \frac{P^2(20;\, s)}{s}ds\right] =$$
$$4 - 2\left[\int_o^r (a_1^2 s^2 + \ldots)ds + r\int_o^\infty \frac{P^2(10;\, s)}{s}ds\right] -$$
$$2\left[\int_o^r (b_1^2 s^2 + \ldots)ds + r\int_o^\infty \frac{P^2(20;\, s)}{s}ds\right] =$$
$$4 - 2\left\{\int_o^\infty \frac{1}{s}\left[P^2(10;\, s) + P^2(20;\, s)\right]ds\right\}r -$$
$$\frac{2}{3}(a_1^2 + b_1^2)r^3 + \ldots =$$
$$4 + v_o r + O(r^3), \text{ for small values of } r,$$
where $v_o = -2\{\qquad\}$.

We will now derive an integral equation involving $Y(\delta r)$ and $Z(r)$.

From the equation 6-13, we see that

6-14 $$\lim_{r\to o} Y(r) = 4$$

6-15 $$Y'(0) = \lim_{r\to o} \frac{Y(r) - 4}{r} = -\lim_{r\to o} \frac{4 - Y(r)}{r}.$$

Now,

6-16 $$\frac{d}{dr}\left[\frac{4-Y(r)}{r}\right] = \frac{1}{r^2}\left[r\left(\frac{-dY(r)}{dr}\right) - \left(4 - Y(r)\right)\right] =$$
$$-\frac{1}{r^2}\left[r\frac{dY(r)}{dr} + 4 - Y(r)\right] =$$
$$-\frac{4 - Z(r)}{r^2}.$$

Integrating this equation, we get

$$6\text{-}17 \qquad -\int_0^{\delta r} \frac{4 - Z(r)}{r^2}dr = \int_{r=0}^{r=\delta r} d\left[\frac{4 - Y(r)}{r}\right] =$$

$$\lim_{h\to o} \frac{4 - Y(r)}{r}\Bigg|_{r=h}^{r=\delta r} =$$

$$\frac{4 - Y(\delta r)}{\delta r} - \lim_{h\to o} \frac{4 - Y(h)}{h} =$$

$$\frac{4 - Y(\delta r)}{\delta r} + Y'(0).$$

Our desired equation is then

$$6\text{-}18 \qquad -Y'(0) = \frac{4 - Y(\delta r)}{\delta r} + \int_0^{\delta r} \frac{4-Z(r)}{r^2}dr \quad .$$

7. STARTING THE OUTWARD INTEGRATION OF THE RADIAL WAVE FUNCTIONS

The equation

$$7\text{-}1 \qquad \left[d^2/dr^2 + (2/r)Y(10;\, r) - \epsilon_{10}\right]P(10;\, r) = 0$$

is to be solved subject to the conditions

$$7\text{-}2 \qquad P(10;\, 0) = 0$$

$$P(10;\, r) \to 0 \text{ as } r \to \infty$$

$$7\text{-}3 \qquad \int_0^{\infty} P^2(10;\, s)ds = 1.$$

Generally speaking, we can not find solutions of equation 7-1 which satisfy conditions 7-2 and 7-3 for an arbitrary value of ϵ_{10}. More precisely, the equation 7-1 has solutions satisfying these conditions only for special values of ϵ_{10} which are called eigenvalues. The fact that the solution of 7-1 must be calculated numerically makes the

eigenvalue problem particularly awkward in this instance. The solution of equation 7-1 must be calculated with an assigned value of ϵ_{10} before we commence, but we are unable to determine ϵ_{10} until we finish.

We omit the label 10 and denote the function by P. We are going to determine P numerically at an evenly spaced set of points, $x_n = nh$ where h is a fixed positive number. We denote by P(n) the value of P at x_n, that is,

7-4 $$P(n) = P(x_n) = P(nh)$$
$$P(n+1) = P\left[(n+1)h\right] = P(x_n + h)$$
$$P(n-1) = P(x_n - h)$$

Assuming the validity of a Taylor series expansion of P, we find that P"(n) is approximately equal to

$$\left[P(n+1) - 2P(n) + P(n-1)\right]/h^2.$$

We use this expression to replace equation 7-1 by

7-5 $$\left[P(n+1) - 2P(n) + P(n-1)\right]/h^2 = \epsilon P(n) - (2/nh)Y(n)P(n).$$

We are able to determine two recursion relations from this equation

7-6 $$P(n+1) = \left[2 + \epsilon h^2 - (2h/n)Y(n)\right]P(n) - P(n-1), \text{ and}$$

7-7 $$P(n-1) = \left[2 + \epsilon h^2 - (2h/n)Y(n)\right]P(n) - P(n+1)$$

Thus, if we know P(n-1), P(n), and ϵ, we are able to calculate P(n+1) by equation 7-6. While if we know P(n+1), P(n), and ϵ we are able to calculate P(n-1) by equation 7-7. Consequently, we are able to use 7-6 to calculate outward from the origin and 7-7 to calculate inward from infinity.

The usual result is that an inward integration and an outward integration do not agree at some point r_o where they should meet smoothly. This lack of match enables one to refine an initial guess at the value of ϵ.

In order to use equation 7-6, one must have starting values for P(0) and P(1). We have the value, P(0) = 0, but we have no value of P(1). A standard method of starting such a solution is by means of a Taylor series expansion about the origin. We now concern ourselves with starting the outward solution.

Our basic assumption is that the equation 7-1,

$$\left[d^2/dr^2 + (2/r)Y(10;\ r) - \epsilon\right]P(r) = 0,$$

has a solution of the form

7-8 $$P(r) = a_o r^m + \ldots + a_n r^{m+n} + \ldots,$$

from which it follows that

7-9 $$P''(r) = (m-1)ma_o r^{m-2} + \ldots + (m+n-1)(m+n)a_n r^{m+n-2} + \ldots$$

$$(8/r)P(r) = 8a_o r^{m-1} + \ldots + 8a_n r^{m+n-1} + \ldots$$

$$\left[2v_o(10) - \epsilon\right]P(r) =$$

$$\left[2v_o(10) - \epsilon\right]a_o r^m + \ldots + \left[2v_o(10) - \epsilon\right]a_n r^{m+n} + \ldots \quad .$$

We now rewrite equation 7-1 as

7-10 $$\left\{d^2/dr^2 + (8/r) + \left[2v_o(10) - \epsilon\right] + 0(r^3)\right\}P(r) = 0$$

where we have replaced Y(10; r) by the approximation

7-11 $$Y(10;\ r) = 4 + rv_o(10) + 0(r^3).$$

We substitute the power series P(r) into 7-10 and determine the coefficients of the lower powers of r.

COEFFICIENT (r^{m-2}):

$$m(m-1)a_o$$

The vanishing of this expression requires $a_o = 0$ or $m = 0$ or $m = 1$. The only acceptable condition is $m = 1$. Thus we see that the power series for P(r) is of the form, $a_o r + \ldots + a_n r^{n+1} + \ldots$.

COEFFICIENT (r^{m-1}):

$$[m(m+1)a_1 + 8a_o]$$

The vanishing of this coefficient requires that $a_1 = -8a_o/2 = -4a_o$.

COEFFICIENT (r^m):

$$(m+1)\ (m+2)a_2 + 8a_1 + [2v_o(10) - \epsilon]a_o$$

The vanishing of this coefficient requires that

$$6a_2 - 32a_o + [2v_o(10) - \epsilon]a_o = 0,$$

from which it follows that

$$a_2 = (32 - [2v_o(10) - \epsilon])a_o/6.$$

COEFFICIENT (r^{m+1}):

$$(m + 2)\ (m + 3)a_3 + 8a_2 + [2v_o(10) - \epsilon]a_1$$

The vanishing of this coefficient requires that

$$12a_3 + 8a_2 + [2v_o(10) - \epsilon]a_1 = 0$$

from which it follows that

$$a_3 = 2(2[2v_o(10) - \epsilon] - 16)a_o/9.$$

Thus we determine a power series expansion of P(10; r) of the form

7-12 $$P(10; r) = a_o r(1 - 4r + (32 - [2v_o(10) - \epsilon])r^2/6 + 2(2[2v_o(10) - \epsilon] - 16)r^3/9 + 0(r^4)).$$

The power series expansion of P(20; r) differs only in the replacement of the expression $[2v_o(10) - \epsilon]$ by the expression $[2v_o(20) - \epsilon]$. We note that these terms, in each instance, arise from one of the power series

7-13 $Y(10; r) = 4 + v_o(10)r + 0(r^3)$

7-14 $Y(20; r) = 4 + v_o(20)r + 0(r^3)$.

Thus $v_o(10)$ and $v_o(20)$ are the values of the derivatives of these functions at the origin. These derivatives can be determined from the numerical values of Y(10; r) and Y(20; r) which are calculated from the values of these functions determined numerically. We have three equations

7-15 $dY_o/dr = (1/r)\,[Y_o(10, 10; r) - Z_o(10, 10; r)\,]$

7-16 $dY_o/dr = (1/r)\,[Y_o(20, 20; r) - Z_o(20, 20; r)\,]$

7-17 $dY/dr = (1/r)\,[Y(r) - Z(r)\,]$.

We use the general formula (Hildebrand, page 82)

7-18 $v_o(n\ell) = [-3Y(n\ell; 0) + 4Y(n\ell; \delta r) - Y(n\ell; 2\delta r)]/(2\delta r)$

to determine $v_o(10)$ and $v_o(20)$.

Hartree recommends that equations 7-15, 7-16, and 7-17 be integrated separately, numerically of course; then Y(10; r) and Y(20; r) are determined from these by the relations

7-19 $Y(10; r) = Y(r) + Y_o(10,10; r)$, and

7-20 $Y(20; r) = Y(r) + Y_o(20,20; r)$.

8. STARTING THE INWARD INTEGRATION OF THE RADIAL WAVE FUNCTIONS

To start the inward integration suppose that R is sufficiently large so that the contribution for r > R is small enough to be disregarded. Then we may start the inward integration ar r = R. We write the equation as

8-1 $P'' = F(r)P$

where F(r) is certainly positive in the neighborhood of r = R. If F(r) is varying slowly, an approximate solution of this equation is

8-2 $P \sim F^{-1/4}[A\exp(+\int F^{1/2}dr) + B\exp(-\int F^{1/2}dr)\ ]$

and we require the solution that increases, roughly exponentially, as r decreases. The values at three equally spaced values of r will be approximately in geometrical progression.

Suppose for the moment that they are in exact geometrical progression and let

8-3 $P(R + \delta r) = A/(1+x)$,

8-4 $P(R) = A$, and

8-5 $P(R - \delta r) = A(1+x)$.

Then

8-6 $(\delta P)_+ = \dfrac{A}{(1+x)} - A$

and

8-7 $(\delta P)_- = A - A(1+x)$,

so that

8-8 $\delta^2 P(R) = \dfrac{A}{(1+x)} - A - (A - A(1+x)) = A/(1+x) - 2A + A(1+x) =$

$$\frac{A-2A-2Ax+A+2Ax+Ax^2}{1+x}$$

$$8\text{-}9 \quad \delta^2 P(R) = \frac{Ax^2}{(1+x)} .$$

But since $P(R) = A$, we have

$$8\text{-}10 \quad P''(R) = F(R)P(R) = AF(R).$$

We have already made the assumption that P has a power series expansion, so that

$$8\text{-}11 \quad P(n+1) = P(n) + P'(n)\delta r + \frac{(\delta r)^2}{2!}P''(n) + \frac{(\delta r)^3}{3!}P'''(n) + 0(\delta r^4)$$

and

$$8\text{-}12 \quad P(n-1) = P(n) - P'(n)\delta r + \frac{(\delta r)^2}{2!}P''(n) - \frac{(\delta r)^3}{3!}P'''(n) + 0(\delta r^4).$$

Hence

$$8\text{-}13 \quad P(n+1) + P(n-1) = 2P(n) + P''(n)\,(\delta r)^2 + 0(\delta r^4),$$

or

$$8\text{-}14 \quad P(n+1) - 2P(n) + P(n-1) = P''(n)\,(\delta r)^2 + 0(\delta r^2).$$

But

$$8\text{-}15 \quad \delta^2 P(n) = (P(n+1) - P(n)) - (P(n) - P(n-1)) =$$

$$P(n+1) - 2P(n) + P(n-1),$$

which implies that

$$8\text{-}16 \quad \delta^2 P(R) = P''(R)\,(\delta r)^2 + 0(\delta r^4) = AF(R)\,(\delta r)^2 + 0(\delta r^4).$$

Neglecting the $0(\delta r^4)$ term in 8-16 and substituting the value of $\delta^2 P(R)$ given by equation 8-16 into equation 8-9 we get

$$8\text{-}17 \quad AF(R)\,(\delta r)^2 = \frac{Ax^2}{(1+x)}$$

or

$$8\text{-}18 \quad x^2 = (1+x)\,F(R)\,(\delta r)^2.$$

Obviously, this equation 8-18 is quadratic in x and therefore has a formal, elementary solution by the quadratic formula. However it is often more convenient to find the proper value of x by the use of the iterative formula:

8-19 $x_{i+1} = [(1+x_i)F(R)\ (\delta r)^2]^{1/2}$.

Since x is to have a small value it is often convenient to start the iteration process of equation 8-19 by $x_o = 0$. If this iteration process does not "settle down" to some reasonable value for x, it is assumed that the increments δr are too large. The increments are decreased and the iteration process is repeated, until a satisfactory convergence is obtained.

Once x has been determined and a value for A has been selected, it is a matter of arithmetic to evaluate the starting values.

8-3 $P(R+\delta r) = \frac{A}{(1+x)}$,

8-4 $P(R) = A$, and

8-5 $P(R-\delta r) = A(1+x)$.

9. PREDICTION OF THE NEW EIGENVALUES

In general, the outward and inward integrations will not be in agreement when first performed. Consequently, we must vary the parameter ϵ for a closer matching.

Consider

$$9\text{-}1 \quad \left[\frac{d^2}{dr^2} + \frac{2Y(r)}{r} - \epsilon\right] P = 0.$$

Then

$$9\text{-}2 \quad \left[\frac{d^2}{dr^2} + \frac{2Y(r)}{r} - (\epsilon + \Delta\epsilon)\right] (P + \Delta P) = 0$$

or

$$9\text{-}3 \quad \left[\frac{d^2}{dr^2} + \frac{2Y(r)}{r} - \epsilon\right] P + \left[\frac{d^2}{dr^2} + \frac{2Y(r)}{r} - \epsilon\right] \Delta P -$$

$$P\Delta\epsilon - \Delta\epsilon\Delta P = 0.$$

By observing that the first term is equal to zero and neglecting the last term, we have

$$9\text{-}4 \quad \left[\frac{d^2}{dr^2} + \frac{2Y(r)}{r} - \epsilon\right]\Delta P = P\Delta\epsilon.$$

Multiplying this equation by P and the original one by $-\Delta P$ and adding the two results we have

$$9\text{-}5 \quad P\left[\frac{d^2}{dr^2} + \frac{2Y(r)}{r} - \epsilon\right]\Delta P = P^2\Delta\epsilon$$

$$9\text{-}6 \quad -\Delta P\left[\frac{d^2}{dr^2} + \frac{2Y(r)}{r} - \epsilon\right]P = 0$$

$$9\text{-}7 \quad P\frac{d^2\Delta P}{dr^2} - \Delta P\frac{d^2P}{dr^2} = P^2\Delta\epsilon.$$

Observe that

$$9\text{-}8 \quad \frac{d}{dr}\left(P\frac{d}{dr}\Delta P - \Delta P\frac{dP}{dr}\right) = P\frac{d^2}{dr^2}\Delta P + \frac{dP}{dr}\frac{d\Delta P}{dr} - \frac{d\Delta P}{dr}\frac{dP}{dr} -$$

$$\Delta P\frac{d^2P}{dr^2} = P\frac{d^2\Delta P}{dr^2} - \Delta P\frac{d^2P}{dr^2},$$

and that

$$9\text{-}9 \quad \frac{d}{dr}\Delta P = \frac{d}{dr}(P_2 - P_1) = \frac{dP_2}{dr} - \frac{dP_1}{dr} = \Delta\left(\frac{dP}{dr}\right) = \Delta P'.$$

Now, we have

$$\int_a^b d(P\Delta P' - P'\Delta P) = \int_a^b P^2\Delta\epsilon dr.$$

$$9\text{-}10 \quad (P\Delta P' - P'\Delta P)\Big|_a^b = \Delta\epsilon\int_a^b P^2 dr.$$

For the outward integration,

$$9\text{-}11 \quad P(0) = \Delta P(0) = 0.$$

$$9\text{-}12 \quad (P\Delta P' - P'\Delta P)_{out} = \Delta\epsilon\int_o^{r_o} P_{out}^2 dr.$$

For the inward integration,

$$9\text{-}13 \quad \lim_{r\to\infty} P(r) = \lim_{r\to\infty} \Delta P(r) = 0.$$

$$9\text{-}14 \quad -(P\Delta P' - P'\Delta P)_{in} = \Delta\epsilon \int_{r_o}^{\infty} P_{in}^2 dr.$$

Now,

$$9\text{-}15 \quad \Delta\left(\frac{P'}{P}\right) = \frac{P\Delta P' - P'\Delta P}{P^2}.$$

Hence,

$$9\text{-}16 \quad \Delta\left(\frac{P'}{P_{out}}\right) = \frac{\Delta\epsilon}{P_{out}^2(r_o)} \int_{o}^{r_o} P_{out}^2 dr, \text{ and}$$

$$9\text{-}17 \quad \Delta\left(\frac{P'}{P}\right)_{in} = -\frac{\Delta\epsilon}{P_{in}^2(r_o)} \int_{r_o}^{\infty} P_{in}^2 dr.$$

The criterion for matching the two integrations is

$$9\text{-}18 \quad \left(\frac{P'}{P}\right)_{out} = \left(\frac{P'}{P}\right)_{in} \text{ at } r = r_o.$$

If the above relation does not hold then we seek an increment of ϵ such that

$$9\text{-}19 \quad \left(\frac{P'}{P}\right)_{out} + \Delta\left(\frac{P'}{P}\right)_{out} = \left(\frac{P'}{P}\right)_{in} + \Delta\left(\frac{P'}{P}\right)_{in} \text{ at } r = r_o.$$

Substituting the above expressions we get

$$9\text{-}20 \quad \left(\frac{P'}{P}\right)_{out} + \frac{\Delta\epsilon}{P_{out}^2(r_o)} \int_{o}^{r_o} P_{out}^2 dr = \left(\frac{P'}{P}\right)_{in} - \frac{\Delta\epsilon}{P_{in}^2(r_o)} \int_{r_o}^{\infty} P_{in}^2 dr$$

$$9\text{-}21 \quad \left\{\frac{1}{P_{out}^2(r_o)} \int_{o}^{r_o} P_{out}^2 dr + \frac{1}{P_{in}^2(r_o)} \int_{r_o}^{\infty} P_{in}^2 dr\right\} \Delta\epsilon =$$

$$-\left[\left(\frac{P'}{P}\right)_{out} - \left(\frac{P'}{P}\right)_{in}\right]_{r=r_o}$$

Define

$$9\text{-}22 \quad P_N(r) = \begin{cases} A\dfrac{P_{out}(r)}{P_{out}(r_o)}, & r \le r_o \\ A\dfrac{P_{in}(r)}{P_{in}(r_o)}, & r > r_o, \end{cases}$$

where A is a number such that

$$9\text{-}23 \quad \int_o^\infty P_N^2(r)dr = 1.$$

Observe that $P_N(r_o) = A$.

Now,

$$9\text{-}24 \quad \int_o^{r_o} \left(\frac{P_{out}(r)}{P_{out}(r_o)}\right)^2 dr + \int_{r_o}^\infty \left(\frac{P_{in}(r)}{P_{in}(r_o)}\right)^2 dr = \frac{1}{A^2} \int_o^\infty P_N^2(r)\, dr =$$

$$\frac{1}{A^2} = \frac{1}{P_N^2(r_o)}.$$

Hence,

$$9\text{-}25 \quad \Delta\epsilon = P_N^2(r_o)\left[\left(\frac{P'}{P}\right)_{out} - \left(\frac{P'}{P}\right)_{in}\right]_{r=r_o}.$$

Once $\Delta\epsilon$ is calculated it is added to the old value ϵ to obtain a new value, $\epsilon+\Delta\epsilon$, to be used as the next trial.

10. PROGRAM WRITEUP

It is intended that this section will enable the reader to actually run the program listed in the last appendix. The appendix just mentioned contains both a listing of the complete deck of IBM cards (program, monitor control, and two sets of data) and the output obtained with this deck. Section 11 of this report contains a flow diagram of the major steps in the solution of the problem at hand.

Detailed procedures are, of course, omitted from the flow diagram in order to restrict its length and to convey the logic of the overall program more clearly. Beside each box in the flow diagram is a reference number. These numbers are listed below, followed by more detailed descriptions of the procedures used to accomplish the corresponding steps and/or lists of the numbers (punched in columns 73 through 80) of the program cards, which actually carry out these steps.

Following the references to the flow diagram, we have listed the computed constants used in the program. We have next listed all the arrays used in the program, with a description of the dimensionality requirements and use of each.

The system of numbering the program cards needs some explanation. First of all the program consists of the main program and the eight subroutine subprograms SETUP, NØRM, CALY, CØE, INTEG, STØRE, ERRØR, and RESULT. All cards of the main program have AS (for Atomic Structure) punched in columns

79 and 80, preceded by sequencing numbers. Similarly, each subroutine subprogram has the first two letters of its name punched in columns 79 and 80, preceded by sequencing numbers. The only exception to this rule is in the case of the cards making up the dimension and common statements. These cards appear in identical form in both the main program and each of the subroutines and, hence, have AS in columns 79 and 80 in every instance.

The experienced reader will recognize the monitor control cards by the asterisk (*) punched in column 1. The only monitor control card omitted is the monitor ID card which must be included as the first card of the deck. Otherwise the deck is ready to be run, as it is listed in the appendix. On the IBM 709 (with the monitor system) the control card CARDS CΘLUMN causes the program or subprogram following that card to be punched out in binary card form once it has been compiled. As the deck appears in the listing, all the subroutine subprograms would be punched into binary card form. The program would then be executed, due to the monitor control card XEQ at the beginning of the program. If a compiled binary deck of the main program is also desired the XEQ card should be followed by a monitor control card CARDS CΘLUMN. The data cards must always be preceded by the monitor control card DATA, as in the listing.

Each complete set of data consists of the following cards (there are two complete sets in the listing):

(1) one card containing all those variables listed below under "(1) Input" (format is card 95AS).

(2) NGR (number of $n\ell$-groups in the atom being considered) groups of cards, with each group consisting of the following cards:

(a) One card containing the sequence number of the $n\ell$-group about to be "setup". This number is used only as a check to help insure that the deck has been stacked properly. This number (called NCΘDE in the program) must appear in columns 1 and 2 (format is card 15SE) of the card. All the cards listed under (b) and (c) below should have these columns blank (indicated by 2X in their format statements).

(b) One card containing all those variables listed below under "(2) Input" (format is card 35SE) for that $n\ell$-group being "setup" (i.e. for $n\ell$-group N=NCΘDE).

(c) The number of cards necessary to contain the table of r's for the $n\ell$-group being "setup" (i.e. for $n\ell$-group N=NCΘDE), with four r's per card (format is card 50SE). The number of these cards necessary for $n\ell$-group N=NCΘDE can be easily calculated by taking the integral part of number (IRMAX(N) + 3)/4.

NOTICE that the data cards listed in the appendix have eight words (i.e. numbers) per card instead of four. The even numbered words (i.e. second, fourth, sixth, and eighth) on these cards are corresponding values of the P functions, which we used as initial "guesses", when using another SETUP

subroutine which read in the P's instead of calculating them (see (3) below). With the SETUP subroutine listed in the appendix these P's are completely ignored (see the 8X's in the format).

We now proceed to the explanation of the flow diagram.

(1) Input: (Cards 90AS--95AS)

NAME1 — First 6 letters of alphabetic name of atom under consideration

NAME2 — Second 6 letters of alphabetic name of atom under consideration

NGR — Number of occupied $n\ell$-groups

IDIM — Maximum length of tables as they are dimensioned in the dimension statement

ALPHA — Scaling constant for A_{out}'s

ZTEST — Test factor for agreement of old and new Z(r)'s

TNORM — Test factor in comparing $\int_0^\infty P^2 dr$ with 1.0 to determine if normalization is necessary

TD2P — Test factor multiplying the absolute value of the second derivative (D2P) to be used as the agreement test between the second derivative (D2P) and second difference (DEL2P) in initialization of outward integration for P's

XTEST — Test factor for convergence of iteration determining x for initializing inward integration of P's

PTEST — Test factor for matching P's from inward and outward integrations

(2) Input: (Cards 160AS--170AS and 30SE--35SE)

IRMAX(N) Index indicating the position number in table of R's which is to be considered as infinity for $n\ell$-group N (i.e. index of $R_{max}(N)$)

IRO(N) Index indicating the position number in tables at which inward and outward integrations for P's for $n\ell$-group N are to be checked for match (i.e. index $R_o(N)$)

E(N) Initial "guess" for $\epsilon_{n\ell}$ for $n\ell$-group N

Q(N) Number of electrons in $n\ell$-group N (i.e. $q(n\ell)$)

AIN(N) Value of A_{in} to be used to initialize inward integration of P's for $n\ell$-group N

(3) Input: (Cards 160AS--170AS and 40SE--100SE)

R(N;I) (I=1,2,. . .,IRMAX(N)) Table of r's for $n\ell$-group N

In the example calculation, the initial P's are calculated from equations for hydrogen-like atoms:

$$P(10; r) = 16re^{-4r}$$

and

$$P(20; r) = (8/\sqrt{2})\, r\,(1/2 - r)e^{-2r}$$

(see Eyring, Walter, and Kimball's Quantum Chemistry, Chap. VI). If one wishes to read in the initial starting values of the P's, instead of calculating them, then he has but to replace cards 40SE--100SE with the appropriate cards to do so and recompile subroutine SETUP.

(4) Initialize old Z(r) positions to zero to make Z(r)'s fail the match text (see (9) of flow diagram) the first time through (Part of card 130AS)

REMARK: Entry point A on flow diagram is at statement number 70 in program (card 295AS).

(5) Normalize P(nℓ: r) for nℓ-group N: Calculates $P^2(n\ell;\ r)$ for nℓ-group N. Calculates $\int_{r_J}^{\infty} P^2(n\ell;\ r)dr$ for nℓ-group N. Compares $\int_0^{\infty} P^2(n\ell;\ r)dr$ with 1.0 with criterion TNΘRM (see (1) of flow diagram) to see if normalized. If not normal, then normalizes $P(n\ell;\ r)$ by

$$P(n\ell;\ r)_{nor} = P(n\ell;\ r) \Big/ \left[\int_0^{\infty} P^2(n\ell;\ r)dr\right]^{1/2}$$

and recalculates $P^2(n\ell;\ r)_{nor}$ and normalizes integral by

$$\int_{r_J}^{\infty} P^2(n\ell;\ r)_{nor}dr =$$

$$\left[\int_{r_J}^{\infty} P^2(n\ell;\ r)dr\right] \Big/ \left[\int_0^{\infty} P^2(n\ell;\ r)dr\right] =$$

$$(1.0 - Z_o(n\ell,\ n\ell;\ r_J))$$

(Cards 320AS and 10NΘ -- 85NΘ and also uses 931AS--935AS)

(6) Determine $A_{out}(N)$ to be used to initialize outward integration of $P(n\ell;\ r)$ for nℓ-group N, by setting

$$A_{out}(N) = ALPHA/(\underset{r_J}{\text{Max}} \mid P(n\ell;\ r_J)_{nor} \mid),$$

where ALPHA is a constant (see (1)) (Cards 320AS and 90NΘ--120NΘ)

(7) Calculate $Z_o(n\ell, n\ell; r)$ for $n\ell$-group N by equation

$$Z_o(n\ell, n\ell; r_J) = 1 - \int_{r_J}^{\infty} P^2(n\ell; r)_{nor} dr$$

(Cards 325AS--335AS)

(8) Calculate $Z_{new}(r)$ by the equation

$$Z_{new}(r) = 4 - 2Z_o(10, 10; r) - 2Z_o(20, 20; r)$$

or, in general,

$$Z_{new}(r) = T\Theta TN = \sum_N Q(N) Z_o(N, N; r)$$

(Cards 301AS and 335AS)

(9) Match test on Z(r)'s to see if the old and the new Z(r)'s agree throughout the range of r's to within an amount equal to ZTEST (see (1)) (Cards 359AS--365AS)

(10) Output results: The program prints out title on page, lists the input parameters used in the calculations, gives number of iterations on P's and on ϵ's carried out, gives final values of the ϵ's, and gives, in table form (with headings and iteration numbers included), the successive values of the functions $P(n\ell; r)$, $Z_o(n\ell, n\ell; r)$, $Y_o(n\ell, n\ell; r)$, and $Y(n\ell; r)$, for each $n\ell$-group, followed by Y(r) and Z(r). (Cards 89AS, 171AS--179AS, 370AS--384AS,

5St--75St, and 5RE-440RE. Also depends upon 75AS--87AS, 145AS, 150AS, 340AS, 345AS, 350AS, 420AS, 440AS, and 941AS)

(11) Put new Z(r) in the old Z(r) positions (Cards 390AS--395AS)

(12) Calculate $Y_o(n\ell, n\ell; r)$ for $n\ell$-group N by setting $Y_o(n\ell, n\ell; r)\,|_{r=\infty} = 0$ and integrating inward by means of the equation

$$Y_o(n\ell, n\ell; r - \delta r) =$$

$$\left[\frac{r-\delta r}{r}\right] Y_o(n\ell, n\ell; r) + \left[\frac{\delta r}{r}\right] Z_o(n\ell, n\ell; r-\delta r).$$

A three-point interpolation scheme is used to cross points in the table where interval length changes.

(Cards 400AS, 415AS, and 5CA--35CA)

(13) Calculate Y(r) by setting $Y(r)\,|_{r=\infty} = 0$ and integrating inward by means of the equation

$$Y(r-\delta r) = \left[\frac{r-\delta r}{r}\right] Y(r) + \left[\frac{\delta r}{r}\right] Z(r-\delta r).$$

(Note: actually by proper assignment of storage this was included in the same "loop" as used to calculate Y_o's) Then the Y(r) are multiplied by a constant so that Y(0) = TΘTN (see (1)). (Cards 400AS, 415AS, 5CA--35CA, and 417AS--419AS)

(14) Calculate $Y(n\ell; r)$ for $n\ell$-group N by the equation

$$Y(n\ell; r) = Y_o(n\ell, n\ell; r) + Y(r).$$

(Cards 405AS and 425AS--440AS)

(15) Calculate $v_o(n\ell)$ for $n\ell$-group N by the equation

$$v_o(n\ell) = [-3Y(n\ell; 0) + 4Y(n\ell; \delta r) - Y(n\ell; 2\delta r)]/(2\delta r)$$

(Hildebrand, page 82) (Cards 445AS--450AS)

REMARK: Entry point D on flow diagram is at statement number 120 in program (Card 460AS).

(16) Calculate coefficients of Taylor series for $P(n\ell; r)$ for $n\ell$-group N, to be used to initialize outward integration of $P(n\ell; r)$ (Cards 470AS and 5CΘ--35CΘ)

(17) (Part of cards 475AS--477AS)

(18) (Cards 565AS--575AS)

(19) Test initialization for outward integration for $P(n\ell; r)$ by evaluating the second derivative at $r = \delta r$, by the equation

$$\frac{d^2P}{dr^2}(n\ell; \delta r) = (\epsilon_{n\ell} - 2Y(n\ell; \delta r)/\delta r)\, P(n\ell; \delta r),$$

and comparing it with the second difference (central), with agreement criterion of

$$TD2P\left|d^2(P(n\ell;\ \delta r))/dr^2\right|$$

(Cards 50AS and 580AS--590AS)

(20) (Card 610AS)

(21) Interpolate for $Y(n\ell;\ \delta r)$ using a three-point interpolation scheme

(Card 50AS and part of 580AS)

(22) Interpolate for $Y(n\ell;\ r)$ out to standard interval, using same scheme as in (21)

(Cards 50AS and 635AS--650AS)

(23) Integrate out to standard interval for $P(n\ell;\ r)$ using equation 7-6 (see body of report)

(Cards 655AS, 15IN, and 340IN--360IN)

(24) Integrate for $P(n\ell;\ r)$, from $r = 0$ to $r = R_o(n\ell)$, using equation 7-6 (see body of report) and a three-point interpolation scheme to cross points in the table where interval length changes

(Cards 685AS, 10IN--15IN, and 20IN--160IN)

(25) Initializes inward integration of $P(n\ell; r)$ by calculating the value of x (see section 8 of report) and setting

$$P(n\ell; R_{max}(n\ell)) = A_{in}(n\ell)/(1 + x),$$

$$P(n\ell; R_{max}(n\ell) - \delta r) = A_{in}(n\ell),$$

and

$$P(n\ell; R_{max}(n\ell) - 2\delta r) = A_{in}(n\ell)(1 + x).$$

(Cards 695AS--795AS)

(26) Integrate for $P(n\ell; r)$, from $R_{max}(n\ell)$ to $R_o(n\ell)$, using equation 7-7 (see body of report) and a three-point interpolation scheme to cross points in the table where interval length changes (then sets $P(n\ell; R_{max}(n\ell)) = 0$)

(Cards 800AS, 10IN--15IN, and 165IN--335IN)

(27) Match test on $P(n\ell; r)$, from inward and outward integrations, at $r = R_o(n\ell)$ for $n\ell$-group N. The values of $(P'/P)_{in}\big|_{r=R_o}$ and $(P'/P)_{out}\big|_{r=R_o}$ are compared, with agreement criterion PTEST. (Cards 55AS and 810AS--930AS)

(28) Calculate new ϵ's by method discussed in section 9 of report. Note that the arrays where $P^2(n\ell; r)$ and the integrals $\int_r^\infty P^2(n\ell; s)ds$ are stored are not in use during this portion of the program. Therefore, they have been used to evaluate $P_N(n\ell; r)$, $P_N^2(n\ell; r)$, and $\int_0^\infty P_N^2(n\ell; r)dr$, which are used in making new approximation for $\epsilon_{n\ell}$.

(Cards 937AS--1025AS)

Computed Constants

MAXR = $\max_{N}(IRMAX(N))$ ($MAXR \leq IDIM$)

TΘTN = N (i.e. the total number of electrons in the system)

SQN = N^2 (i.e. = $(T\Theta TN)^2$)

Dimension Requirements and Usage of Arrays

AGP(I) ($I \geq 35$) AuGmented P array, used in integrating out to standard interval for P's, when refinement is necessary in initializing outward integration of P's.

AGR(I) ($I \geq 35$) AuGmented R array, used in above procedure.

AGY(I) ($I \geq 35$) AuGmented Y array, used in above procedure to store interpolated values of $Y(n\ell; r)$.

AIN(I) ($I \geq NGR$) for A_{in}'s used to initialize inward integration of P's (see Input).

AΘUT(I) ($I \geq NGR$) for A_{out}'s used to initialize the outward integration of P's.

C(I,J) ($I \geq NGR$; $J \geq 4$) for Taylor series coefficients used in initializing outward integration of P's for $n\ell$-group I.

E(I) ($I \geq NGR$) for $\epsilon_{n\ell}$ for $n\ell$-group I.

IRMAX(I) ($I \geq NGR$) defined under Input.

IRO(I) ($I \geq$ NGR) defined under Input.

ITER(I) ($I \geq 10$) for ITERation number, used in outputing results.

ΘUT(I,J) ($I \geq 10$; MAXR $\leq J =$ IDIM) used in building tables in outputing results.

P(I,J,K) ($I \geq$ NGR; $J \geq 3$; $K =$ IDIM)

P(I,1,K) ($K = 1, 2, \ldots,$ IRMAX(I)) for $P(n\ell; r_K)$ for $n\ell$-group I

P(I,2,K) ($K = 1, 2, \ldots,$ IRMAX(I)) for $P^2(n\ell; r_K)$ for $n\ell$-group I

P(I,3,K) ($K = 1, 2, \ldots,$ IRMAX(I)) for

$$\int_{r_K}^{\infty} P^2(n\ell; r)dr \text{ for } n\ell\text{-group I}$$

PIN(I) ($I \geq$ NGR) for $(P'/P)_{in}\big|_{r=R_o(I)}$ for $n\ell$-group I

PΘUT(I) ($I \geq$ NGR) for $(P'/P)_{out}\big|_{r=R_o(I)}$ for $n\ell$-group I

PRO(I) ($I \geq$ NGR) for P_{in} at $r = R_o(I)$ for $n\ell$-group I

Q(I) ($I \geq$ NGR) for $q(n\ell)$ for $n\ell$-group I (see Input)

R(I,J) ($I \geq$ NGR; MAXR $\leq J =$ IDIM)

R(I,J) ($J = 1, 2, \ldots,$ IRMAX(I)) for r_J for $n\ell$-group I

VO(I) ($I \geq$ NGR) for $v_o(n\ell)$ for $n\ell$-group I

Y(I,J) ($I \geq$ NGR + 1; MAXR $\leq J =$ IDIM)

Y(I,J) ($I = 1, \ldots,$ NGR; $J = 1, \ldots,$ MAXR) for $Y_o(n\ell, n\ell; r_J)$ for $n\ell$-group I

Y(I,J) (I = NGR + 1; J = 1, ..., MAXR) for $Y(r_J)$

YT(I,J) ($I \geq NGR$; $MAXR \leq J = IDIM$)

YT(I,J) (J = 1, 2, ..., MAXR) for $Y(n\ell; r_J)$ for $n\ell$-group I

Z(I,J) ($I \geq NGR + 2$; $MAXR \leq J = IDIM$)

Z(I,J) (I = 1, ..., NGR; J = 1, ..., MAXR)

for $Z_o(n\ell, n\ell; r_J)$ for $n\ell$-group I

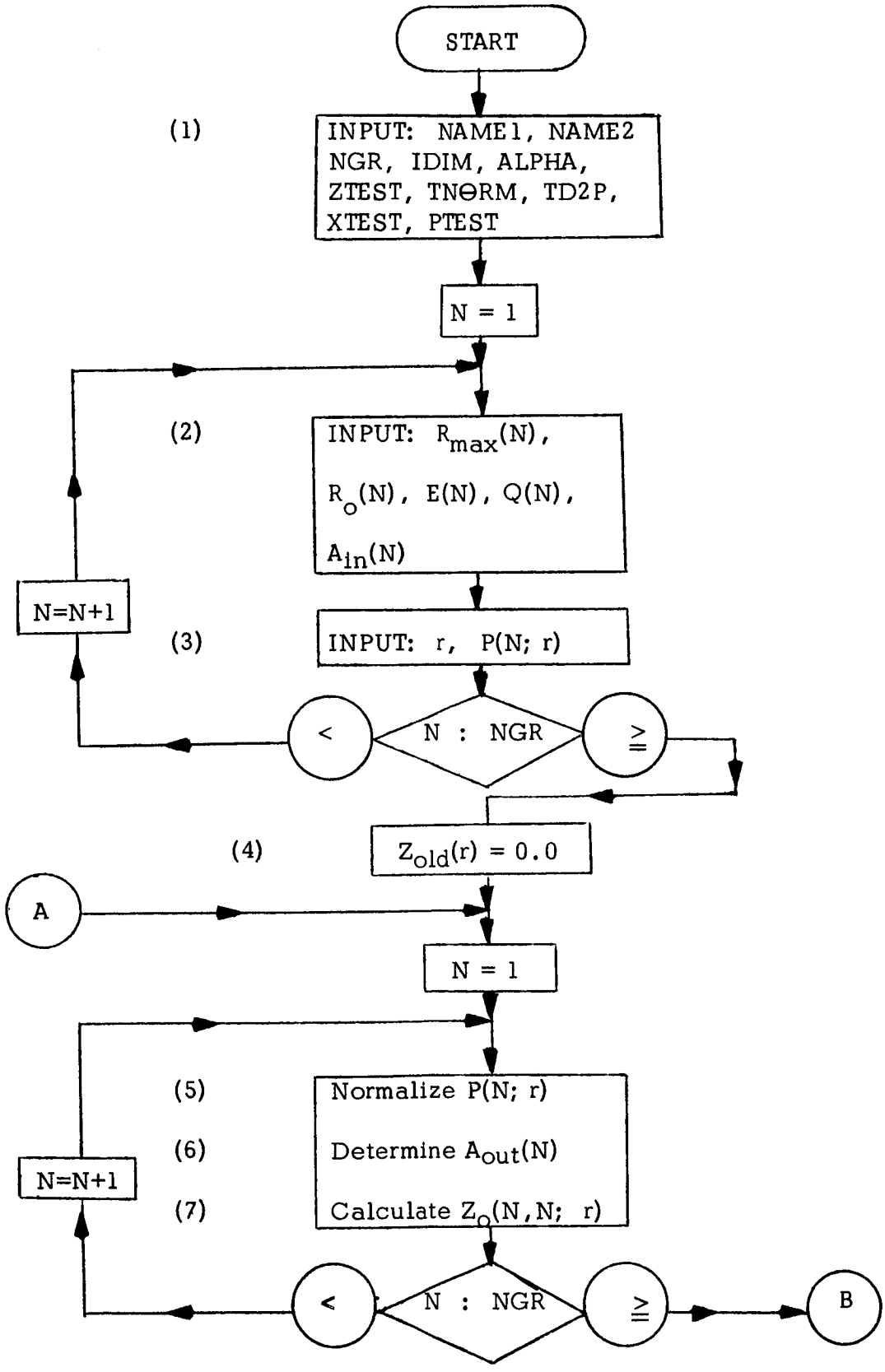
Z(I,J) (I = NGR + 1; J = 1, ..., MAXR)

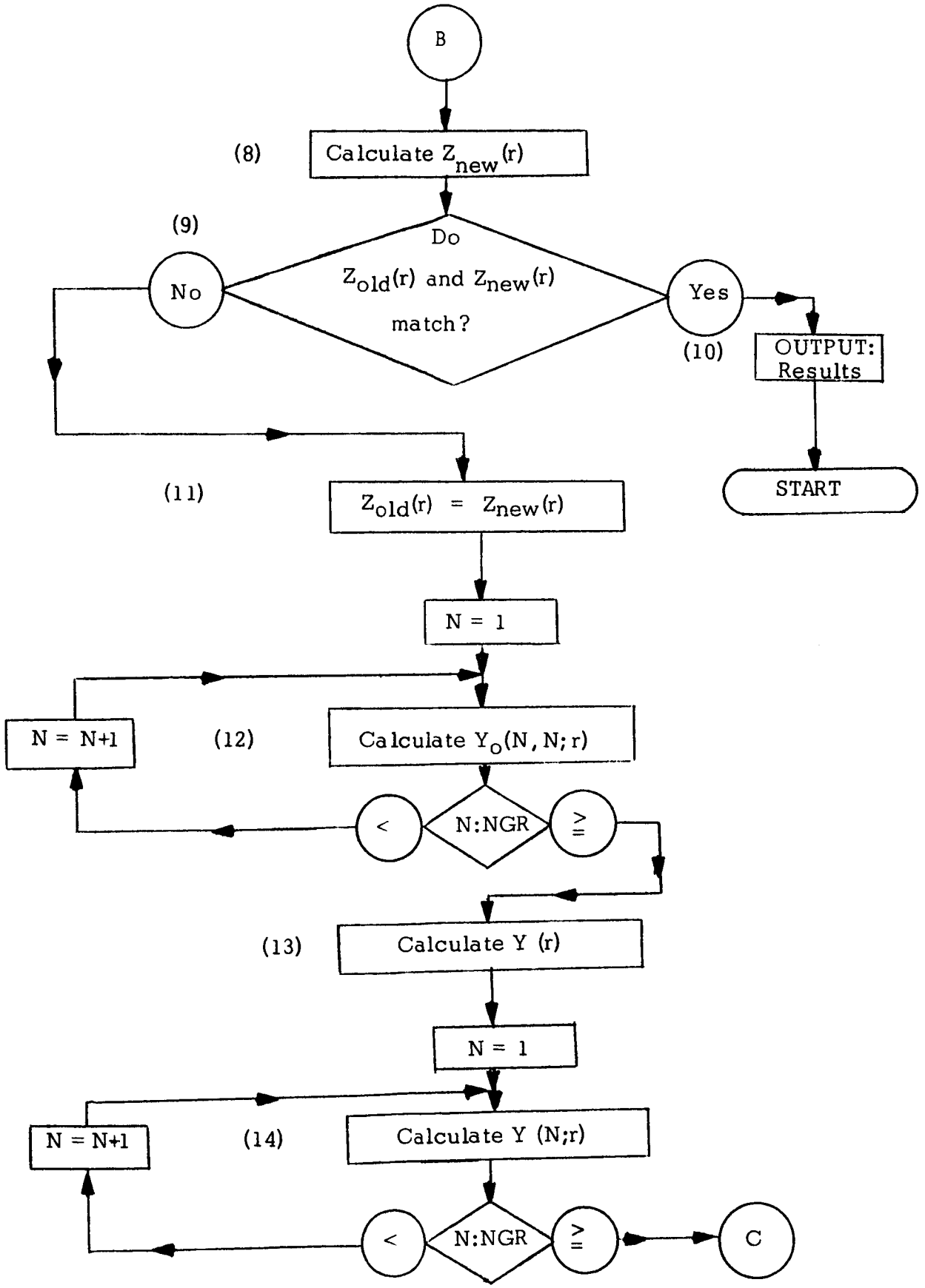
for $Z_{old}(r_J)$ for $n\ell$-group I

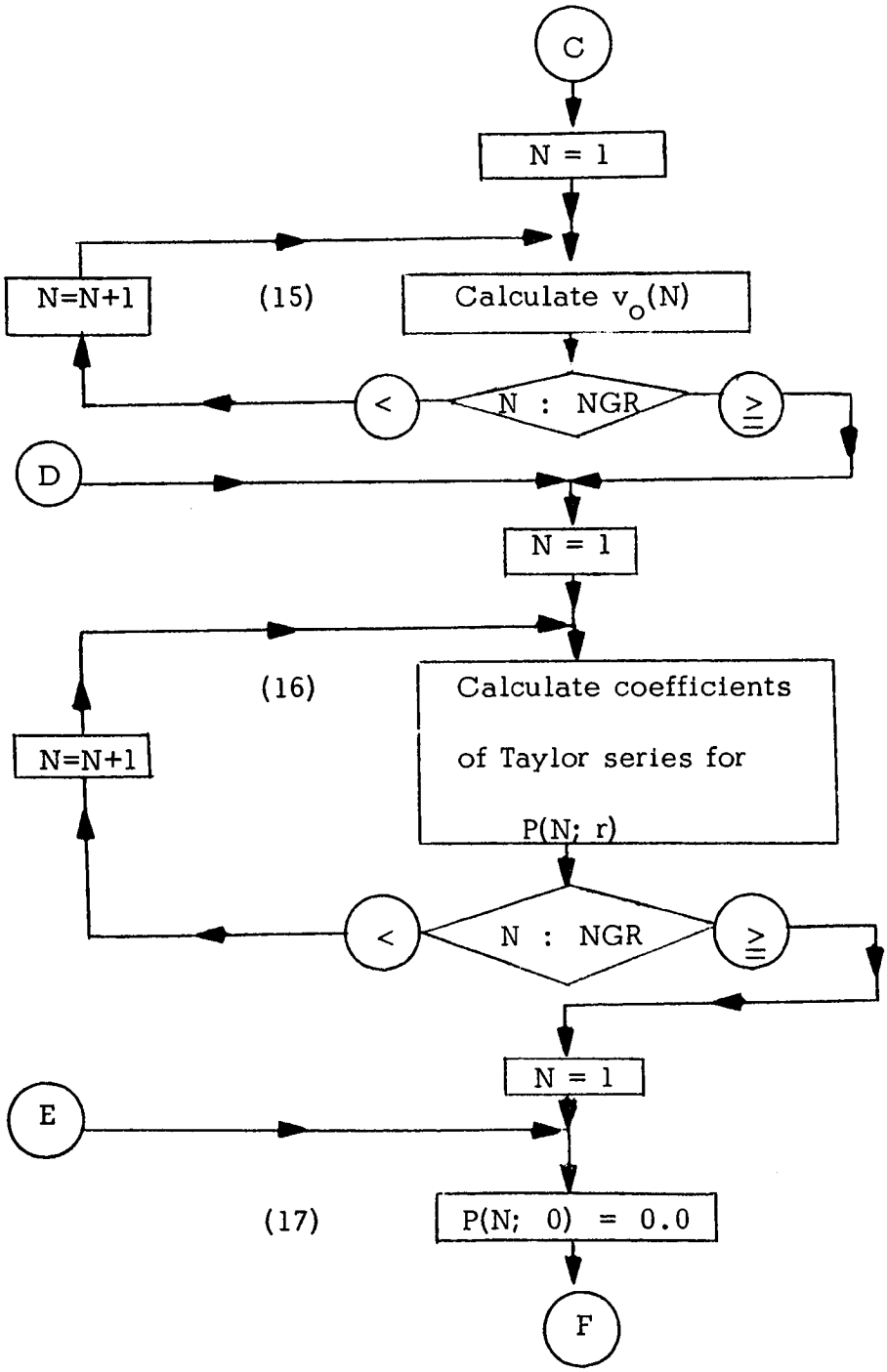
Z(I,J) (I = NGR + 2; J = 1, ..., MAXR)

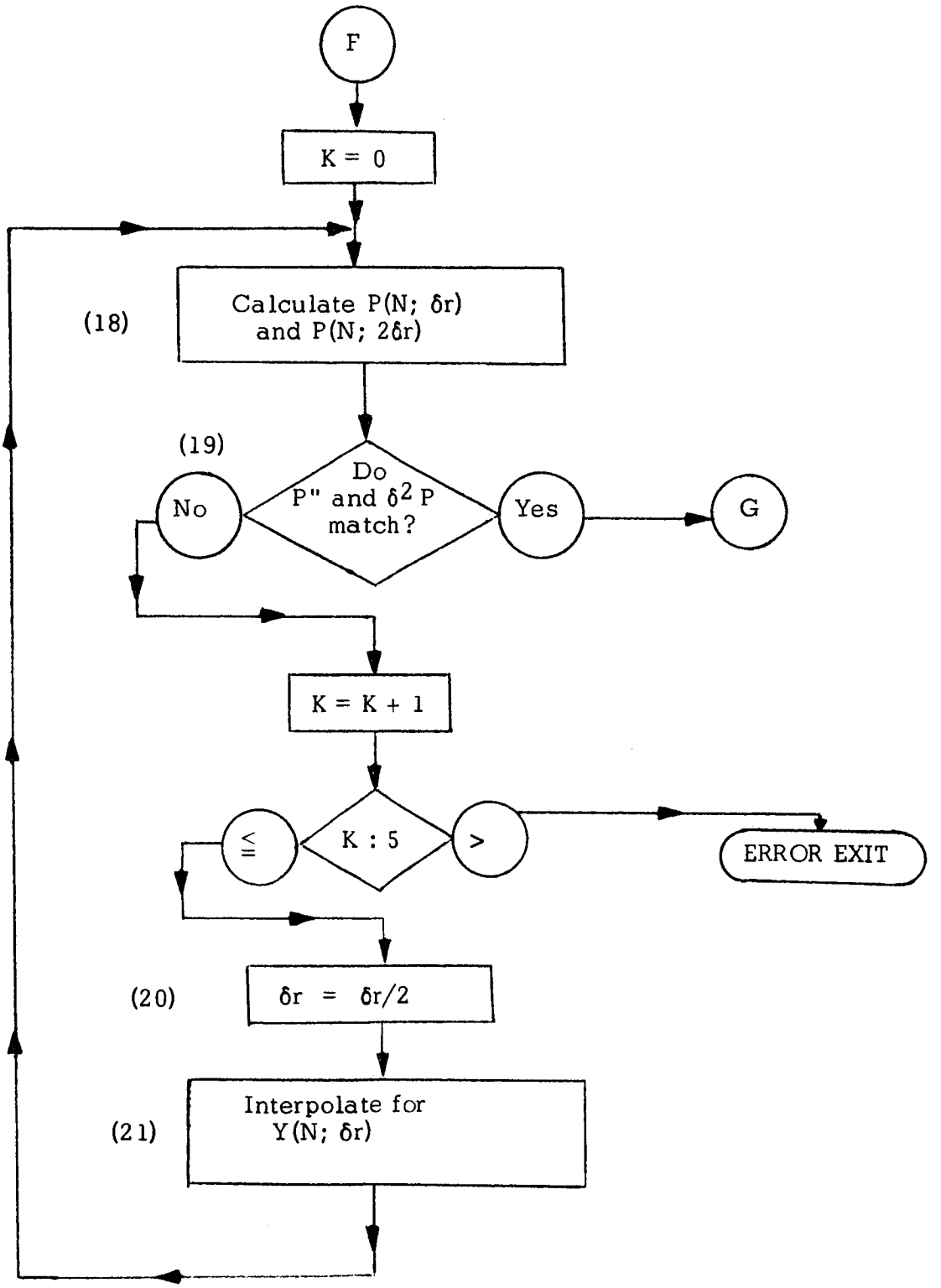
for $Z_{new}(r_J)$ for $n\ell$-group I

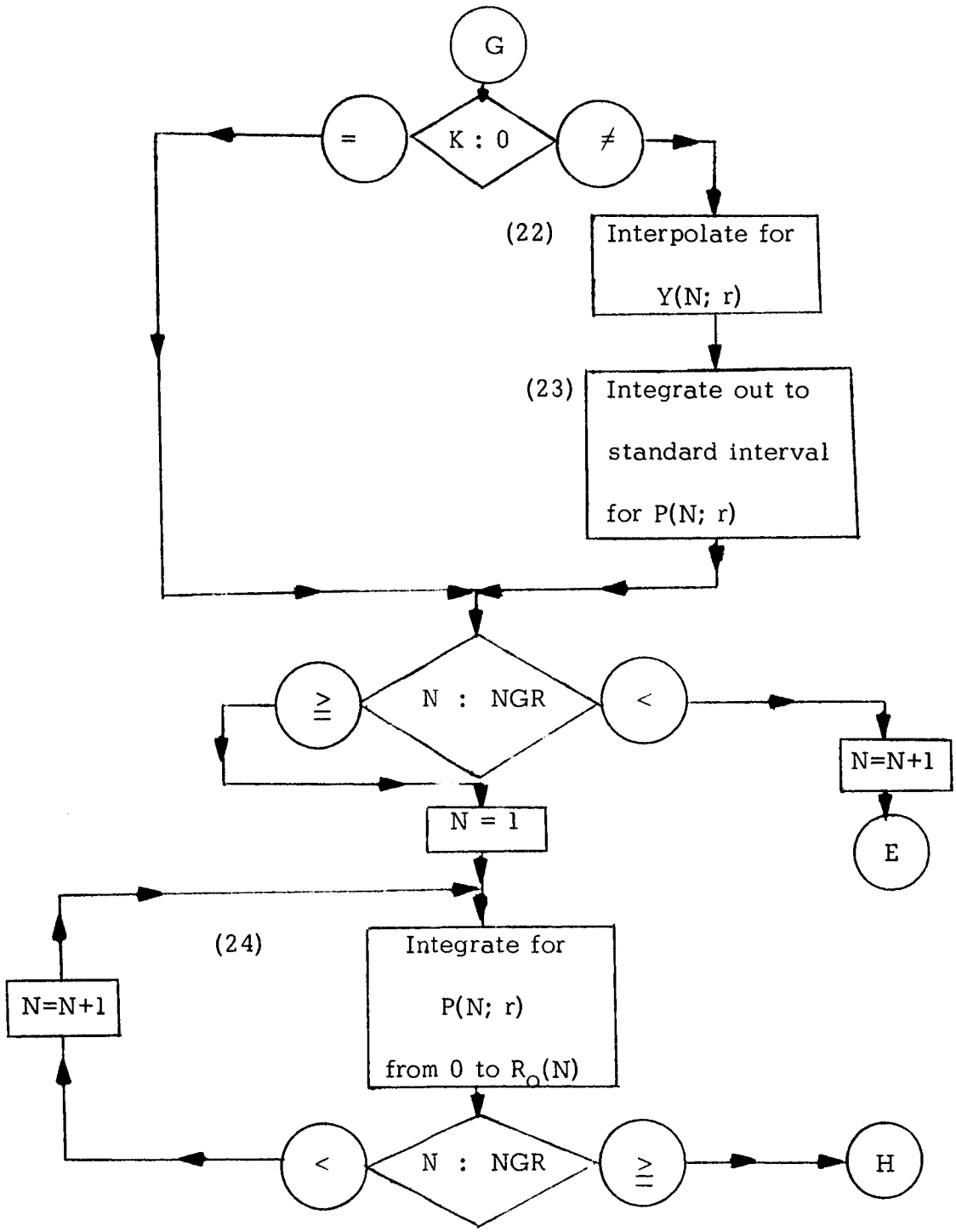
11. FLOW DIAGRAMS

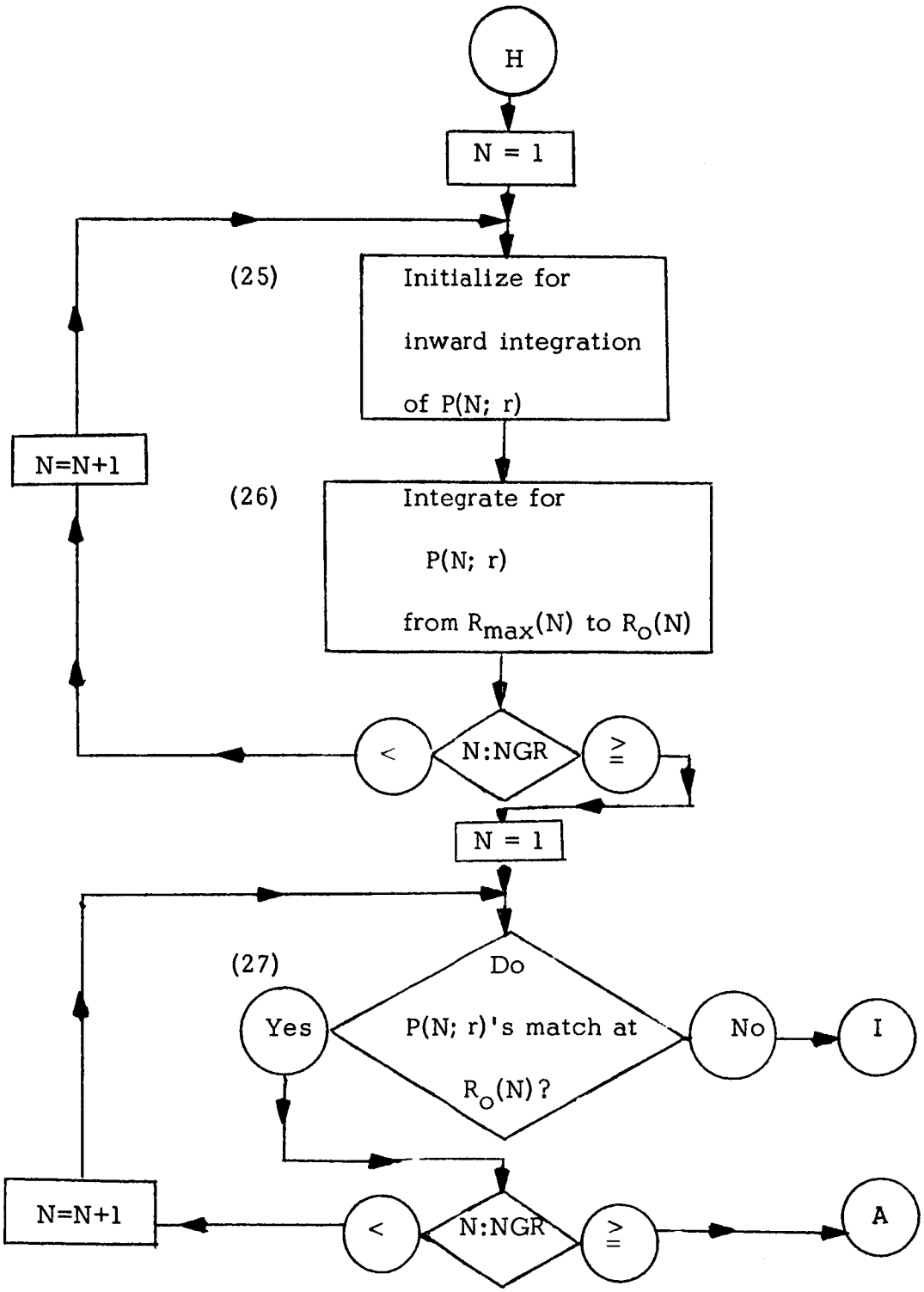


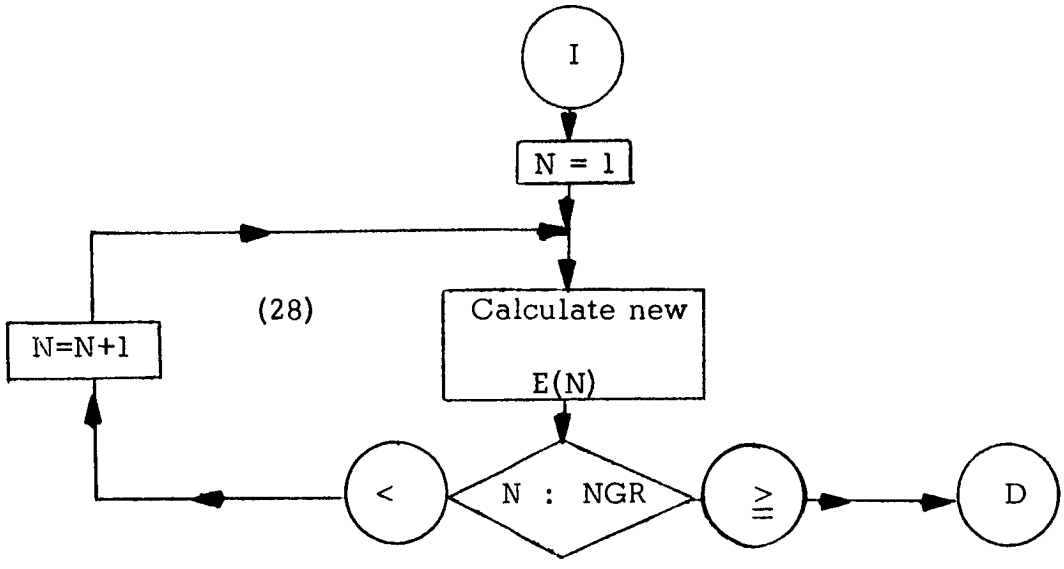

B
(8)
Calculate $Z_{new}(r)$
(9)
Do
$Z_{old}(r)$ and $Z_{new}(r)$
match?
No
Yes
(10)
OUTPUT:
Results
START
(11)
$Z_{old}(r) = Z_{new}(r)$
N = 1
N = N+1
(12)
Calculate $Y_o(N, N; r)$
<
N:NGR
≥
(13)
Calculate Y (r)
N = 1
N = N+1
(14)
Calculate Y (N;r)
<
N:NGR
≥
C


C
N = 1
N=N+1
(15)
Calculate $v_o(N)$
<
N : NGR
≥
D
N = 1
(16)
Calculate coefficients
of Taylor series for
P(N; r)
N=N+1
<
N : NGR
≥
N = 1
E
(17)
P(N; 0) = 0.0
F


F
K = 0
(18)
Calculate P(N; δr) and P(N; 2δr)
(19)
Do P" and δ2 P match?
No
Yes
G
K = K + 1
≤
K : 5
>
ERROR EXIT
(20)
δr = δr/2
(21)
Interpolate for Y(N; δr)


G
K : 0
=
≠
(22)
Interpolate for
Y(N; r)
(23)
Integrate out to
standard interval
for P(N; r)
N : NGR
≥
<
N=N+1
E
N = 1
(24)
Integrate for
P(N; r)
from 0 to R_O(N)
N=N+1
N : NGR
<
≥
H


H
N = 1
(25)
Initialize for inward integration of P(N; r)
N=N+1
(26)
Integrate for P(N; r) from $R_{max}(N)$ to $R_o(N)$
<
N:NGR
≥
N = 1
(27)
Do P(N; r)'s match at $R_o(N)$?
Yes
No
I
N=N+1
<
N:NGR
≥
A


I
N = 1
(28)
Calculate new
E(N)
N=N+1
<
N : NGR
≥
D

12. REFERENCES

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APPENDIX

APPENDIX I

PHYSICAL INTERPRETATION OF Y_K AND Z_K

We recall that with the proper choice of units the potential of a point charge of q units is q/r at a point r units from the charge q. Also the electric field intensity at r is given by $F = -dV/dr = q/r^2$. The sign of the charge q determine the necessary sign adjustments. These basic facts may be used to determine the field F and the potential V of more complicated charge distributions.

We consider a thin ($\cong$ 0 thickness) sphere of radius a which bears a charge of ρ units per unit of surface area. Let P and P' denote two points, the first of which is exterior and the second of which is interior to the sphere. Denote the radii of P and P' by r and r', respectively. We summarize the pertinent facts for this situation.

The <u>charge</u> on the sphere is (1)

$$Q = 4\pi a^2 \rho,$$

The <u>field</u> at the point P is (2)

$$F = 4\pi a^2 \rho / r^2$$

The <u>potential</u> at the point P is (3)

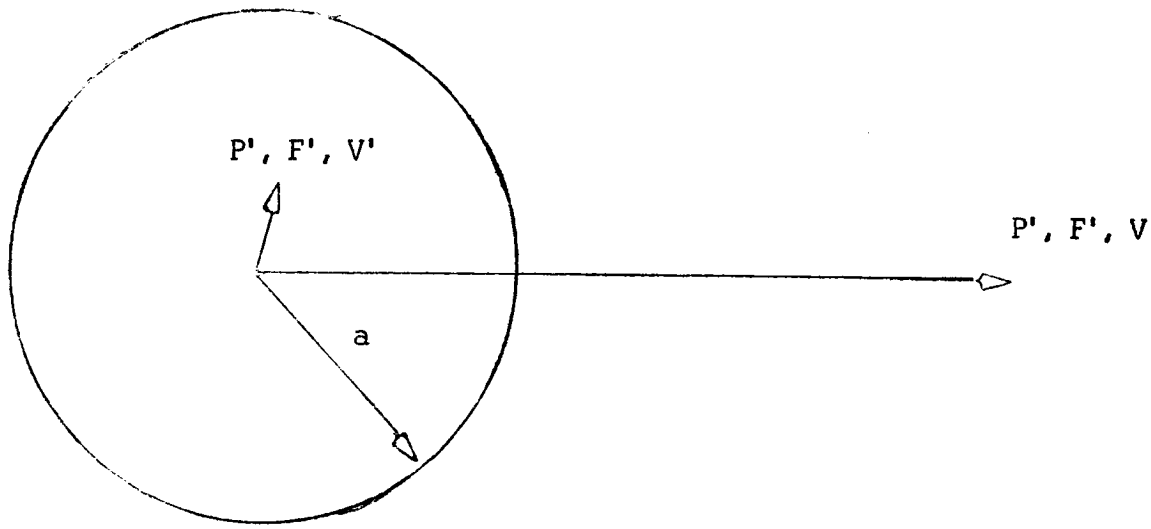
$$V = 4\pi a^2 \rho / r$$

The <u>field</u> at P' is (4)

$$F' = 0$$

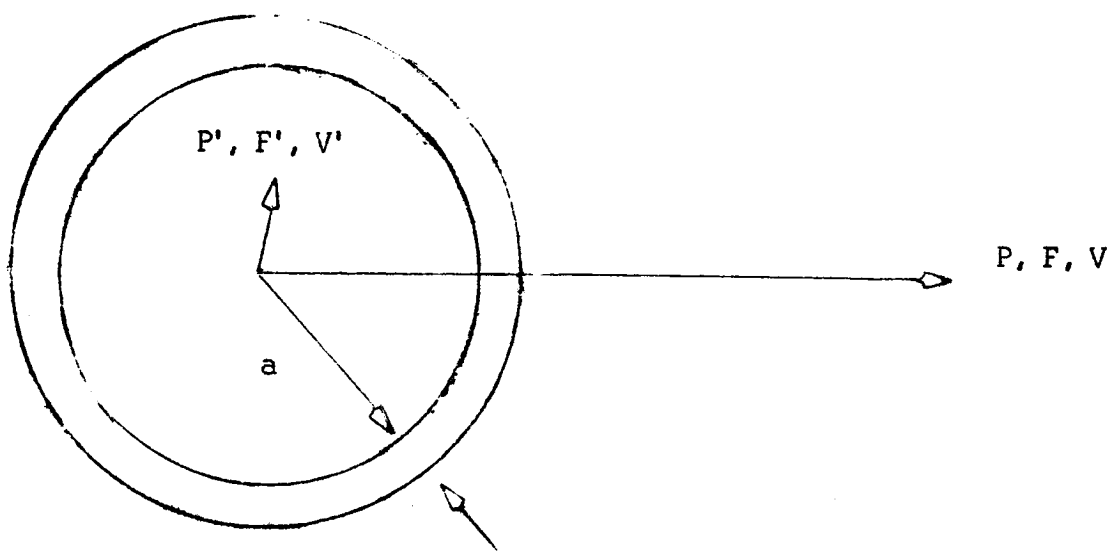
The potential at the point P' is (5)

$$V' = 4\pi a^2 \rho/a = 4\pi a\rho$$



The above diagram is a rough sketch of the situation.

We wish to apply these considerations to a discussion of the terms which appear in the Hartree-Fock equations. Our first observation is that for a thin sphere of radius a and thickness ds, the quantity $P^2(10; a)\, ds/4\pi$ can be considered as playing the role of the charge density function ρ. Consequently, $4\pi\rho$ corresponds to $P^2(10; a)ds$ for a 1s electron associated with $P(10; a)$.



We now recall that the wave function $\psi(10, 0\alpha)$ is given by

$$\frac{\alpha}{2\sqrt{\pi}} \cdot \frac{P(10:r)}{r}$$

The probability that a $\psi(10, 0\alpha)$ electron be observed in a thin sphere of radius a and thickness Δa about the origin is given by

$$\sum \int_a^{a+\Delta a} \int_0^{2\pi} \int_0^{\pi} \frac{\alpha^2}{4\pi} \frac{P^2(10; s)s^2 \sin\theta d\theta d\phi ds}{s^2} =$$

$$\int_a^{a+\Delta a} P^2(10; a)ds \cong P^2(10; a)\Delta a$$

Under many observations, this probability acts like a real charge so that it creates an average potential and field just as though there existed a real charge equal to the probability. We see that the average charge U(s) per unit radius is given by $P^2(10; s)$ for the one electron described by P(10; s). The usual charge density $\rho(s)$ for such a symmetrically distributed charge is given by $\rho(s) = U(s)/4\pi s^2$ or

$$4\pi s^2 \rho(s) = U(s) = P^2(10; s)$$

Thus we are able to discuss the average field and potential of this electron. We have the contribution due to a thin sphere of radius a and thickness ds to be

The charge on the sphere is (1')

$$Q = P(10; s)ds$$

The field at the point P is

$$F = P^2\,(10;\, s)ds/r^2 \qquad (2')$$

The potential at the point P is

$$V = P^2\,(10;\, s)ds/r \qquad (3')$$

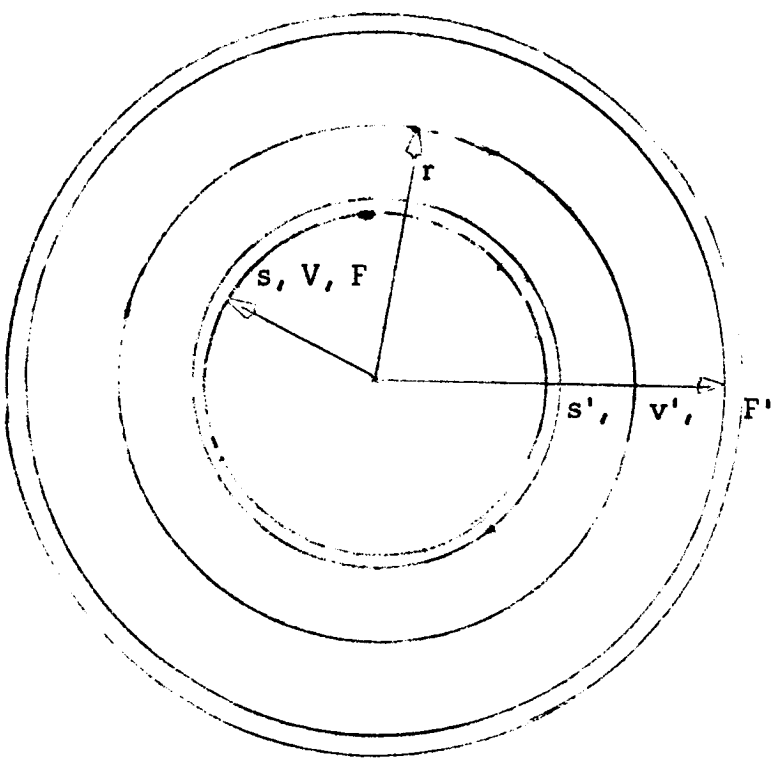
The field at the point P' is (4')

$$F' = 0$$

The potential at the point P' is (5')

$$V' = P^2\,(10;s)ds/s$$

We use these results to calculate the field at a point P with radial coordinate r due to all such shells



$$V = P^2\,(10;\, s)ds/r$$

$$F = P^2\,(10;\, s)ds/r^2$$

$$V' = P^2\,(10;\, s')ds/s'$$

$$F' = 0$$

We find

$$\underline{\text{Potential}} = \int_0^r P^2(10;\, s)ds/r + \int_r^\infty P^2(10;\, s)ds/s$$

$$= Y_o(10,10;\, r)/r$$

$$\underline{\text{Field}} = \int_0^r P^2(10;\, s)ds/r^2 = Z_o(10,10;\, r)/r^2$$

Thus we see that the functions $Y_o(10,10;\, r)$ and $Z_o(10,10;\, r)$ determine the average potential and the average field at r due to a single electron in the 1s shell. In a similar manner, the functions $Y_o(20,20;\, r)$ and $Z_o(20,20;\, r)$ determine the potential at r due to a single electron in the 2s shell.

We now see that if the function Y(r) is defined by

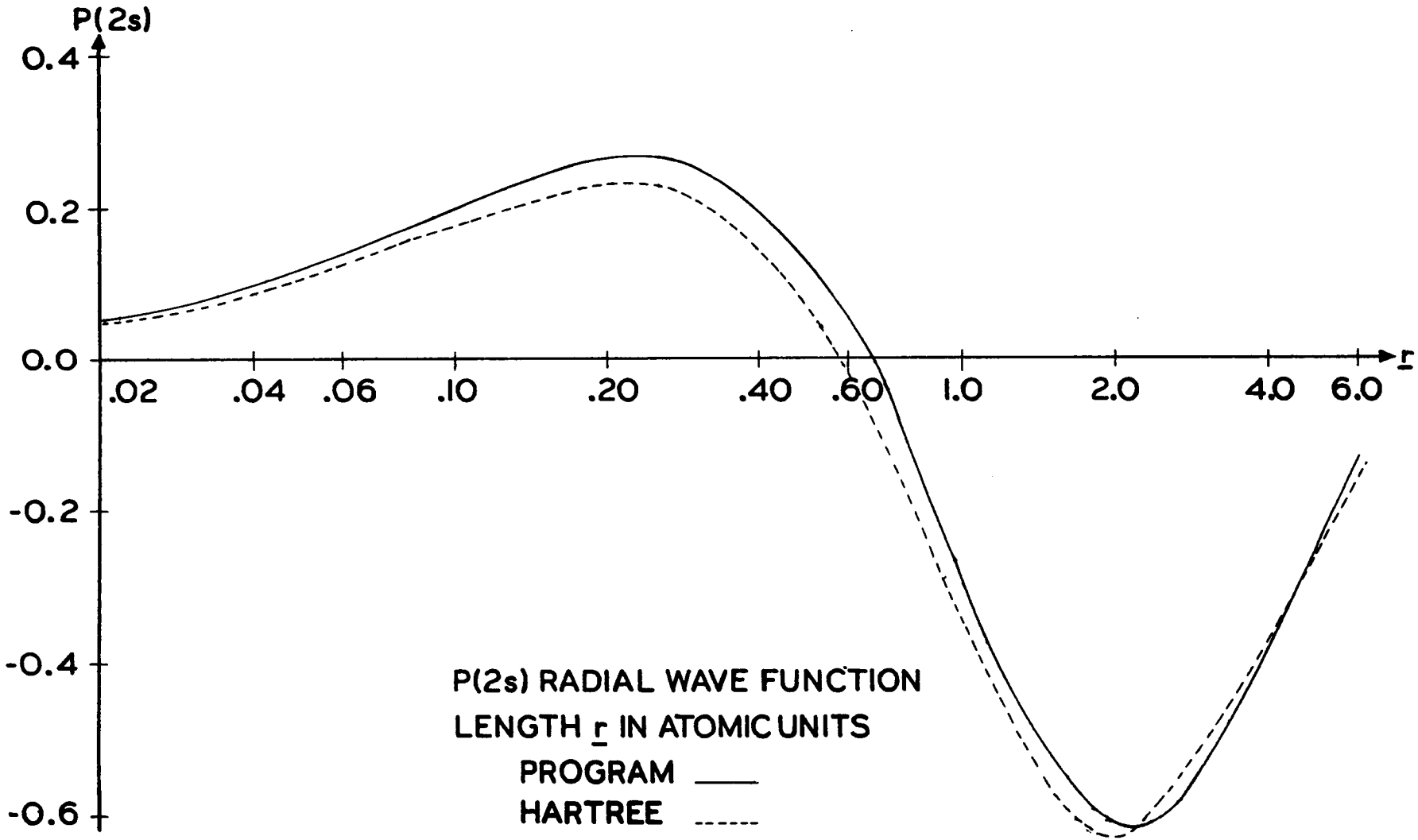
$$Y(r) = 4 - 2Y_o(10,10;\, r) - 2Y_o(20,20;\, r)$$

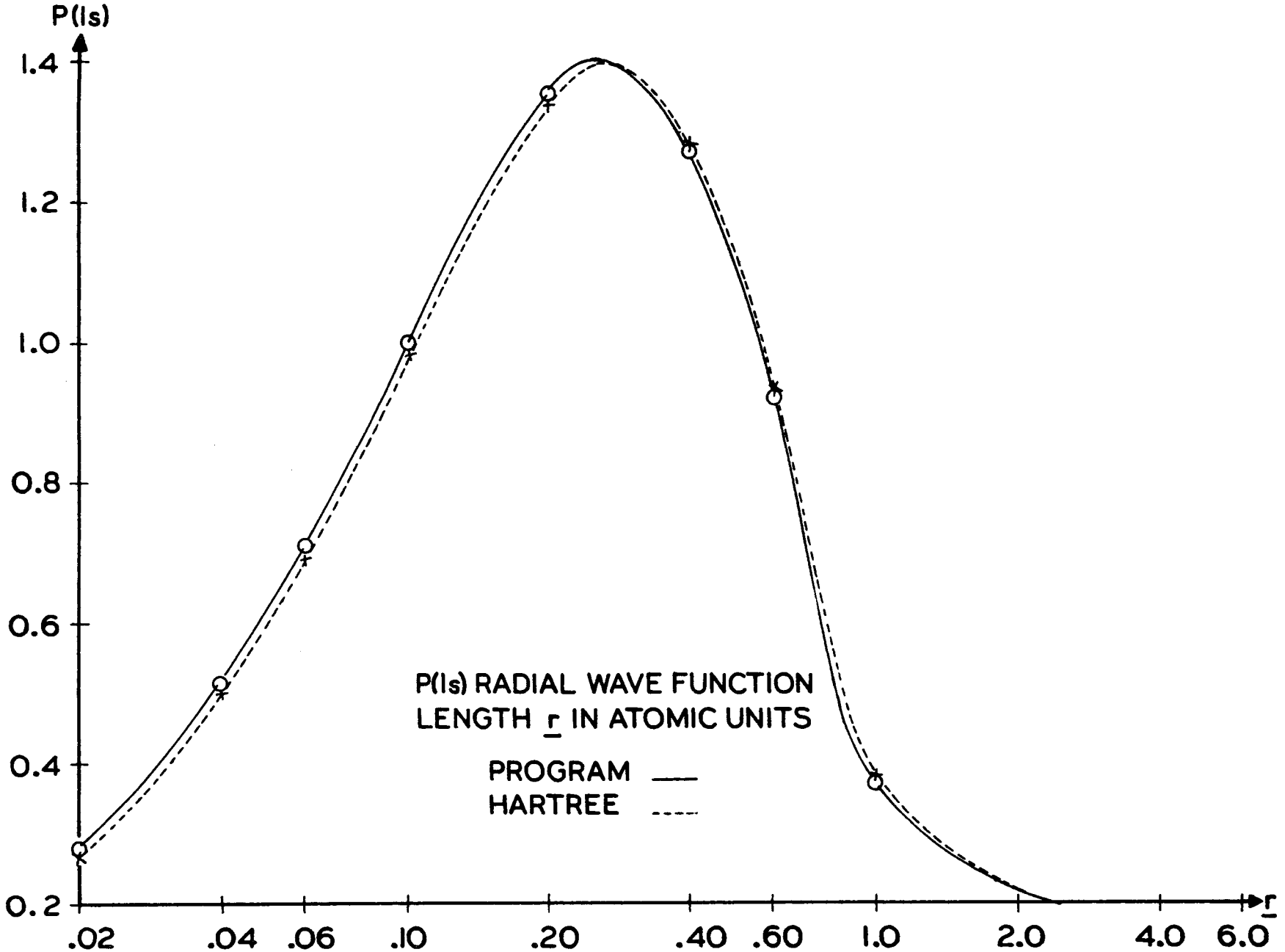
then $\underline{\frac{Y(r)}{r}}$ is the average potential at P due to the nuclear charge and the average charge distribution of both 1s and both 2s electrons. While if

$$Y(10;\, r) = Y(r) + Y_o(10,10;\, r) \text{ and}$$

$$Y(20;\, r) = Y(r) + Y_o(20,20;\, r)$$

then $Y(10;\, r)/r$ and $Y(20;\, r)/r$ are the average potentials seen by a 1s and a 2s electron respectively.


P(2s)
0.4
0.2
0.0
-0.2
-0.4
-0.6
.02
.04
.06
.10
.20
.40
.60
1.0
2.0
4.0
6.0
r
P(2s) RADIAL WAVE FUNCTION
LENGTH r IN ATOMIC UNITS
PROGRAM ____
HARTREE -----


P(1s)
1.4
1.2
1.0
0.8
0.6
0.4
0.2
.02
.04
.06
.10
.20
.40
.60
1.0
2.0
4.0
6.0
r
P(1s) RADIAL WAVE FUNCTION
LENGTH r IN ATOMIC UNITS
PROGRAM
HARTREE

```
*      XEQ
 1000 FORMAT (45H1CALCULATION OF ATOMIC STRUCTURE      CONATSER /// )          5AS
      DIMENSION AGP(35),AGR(35),AGY(35),AIN(2),AOUT(2),C(2,4),E(2),IRMAX     10AS
     1(2),IRO(2),ITER(10),OUT(10,150),P(2,3,150),PIN(2),POUT(2),PRO(2),Q     15AS
     2(2),R(2,150),V0(2),Y(3,150),YT(2,150),Z(4,150)                         20AS
      COMMON AGP,AGR,AGY,AIN,AOUT,C,E,IRMAX,IRO,ITER,OUT,P,PIN,POUT,PRO,     25AS
     1Q,R,V0,Y,YT,Z,ALPHA,D1,D2,D3,D2P,DEL,DEL2P,DNEW,FR,IDIM,IMAX,IMIN,     30AS
     2ITE,ITP,JUMP,K1,K2,K3,KMAX,KMIN,MAXR,NAME1,NAME2,NGR,NGRP1,NGRP2,      35AS
     3P1,PIM2,P1P2,PTEST,R1,R2,R3,SQDEL,SQN,TD2P,TEST,TNORM,TOTN,X1,         40AS
     4XTEST,ZTEST,A,B,X                                                      45AS
      YINTF(X)=(X-R2)*(X-R3)*D1+(X-R1)*(X-R3)*D2+(X-R1)*(X-R2)*D3            50AS
      PRIMEF(X)=A*X+B                                                        55AS
      PRINT 1005,                                                            75AS
 1005 FORMAT (62H MOUNT SCRATCH TAPE ON LOGICAL TAPE UNIT 8 AND PRESS ST     80AS
     1ART KEY ////// )                                                       85AS
      PAUSE 77777                                                            86AS
      REWIND 8                                                               87AS
    3 OUTPUT,1000,                                                           89AS
      INPUT,1010,NAME1,NAME2,NGR,IDIM,ALPHA,ZTEST,TNORM,TD2P,XTEST,PTEST     90AS
 1010 FORMAT (2A6,2I3,6F8.5)                                                 95AS
      NGRP1=NGR+1                                                           100AS
      NGRP2=NGR+2                                                           105AS
      CALL ERASE (P(1,1,1),P(NGR,3,IDIM))                                   110AS
      CALL ERASE (R(1,1),R(NGR,IDIM))                                       115AS
      CALL ERASE (Y(1,1),Y(NGRP1,IDIM))                                     120AS
      CALL ERASE (YT(1,1),YT(NGR,IDIM))                                     125AS
      CALL ERASE (Z(1,1),Z(NGRP2,IDIM))                                     130AS
      ITP=0                                                                 145AS
      ITE=0                                                                 150AS
      MAXR=1                                                                155AS
      DO 5 N=1,NGR                                                          160AS
      CALL SETUP(N)                                                         165AS
    5 MAXR=XMAXOF(MAXR,IRMAX(N))                                            170AS
      OUTPUT,1012,NAME1,NAME2,NGR,IDIM,ALPHA,ZTEST,TNORM,TD2P,XTEST,PTES    171AS
     1T,( N,IRMAX(N),N,IRO(N),N,Q(N),N,AIN(N),N=1,NGR)                      172AS
 1012 FORMAT (35H0INPUT FOR NEXT  CALCULATIONS WERE /// 7H0ATOM = 2A6,/     173AS
     1 6H0NGR = I3,/7H0IDIM =I3,/8H0ALPHA =F9.6,/8H0ZTEST =F9.6,/8H0TNOR    174AS
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     2M = F9.6,/7H0TD2P =F9.6,/8H0XTEST = F9.6,/8H0PTEST = F9.6,/( 7H0IR    175AS
     3MAX( I3,2H)= I4,/ 5H0IR0( I3,2H)= I4,/ 3H0Q( I3,2H)= F10.4,/ 5H0AI    176AS
     4N( I3,2H)= F10.6,   ) )                                               177AS
      OUTPUT,1013,(N,E(N),N=1,NGR)                                          178AS
1013 FORMAT ( 3H0E( I2, 4H )= E13.6)                                        179AS
      TOTN=0                                                                179AS
      DO 10 N=1,NGR                                                         180AS
   10 TOTN=TOTN+Q(N)                                                        185AS
      SQN=TOTN*TOTN                                                         190AS
      DO 15 N=1,NGR                                                         195AS
      IF (MAXR-IRMAX(N)) 20,20,15                                           200AS
   15 CONTINUE                                                              205AS
      CALL ERROR(1,0,0,0)                                                   210AS
      GO TO 87                                                              212AS
   20 M=N                                                                   215AS
      DO 60 N=1,NGR                                                         220AS
      IF (N-M) 25,60,25                                                     225AS
   25 IMAX=IRMAX(N)                                                         230AS
      DO 35 I=1,IMAX                                                        235AS
      IF (R(N,I)-R(M,I)) 30,35,30                                           240AS
   30 CALL ERROR(2,N,M,I)                                                   245AS
      GO TO 87                                                              247AS
   35 CONTINUE                                                              250AS
      IF (P(N,1,IMAX)) 40,45,40                                             255AS
   40 CALL ERROR (3,N,0,0)                                                  260AS
      GO TO 87                                                              262AS
   45 IF (IMAX-MAXR) 50,60,60                                               265AS
   50 DO 55 I=IMAX,MAXR                                                     270AS
   55 R(N,I)=R(M,I)                                                         275AS
   60 CONTINUE                                                              280AS
      IF (P(M,1,MAXR)) 65,70,65                                             285AS
   65 CALL ERROR(4,M,0,0)                                                   290AS
      GO TO 87                                                              292AS
   70 ITP=ITP+1                                                             295AS
      IF (SENSE SWITCH 6) 71,72                                             296AS
   71 PRINT 1015,ITP                                                        297AS
1015 FORMAT (21H BEGINNING ITERATION I3,11H ON THE P-S /////  )             298AS
```

```
   72 DO 73 I=1,IDIM                                                          300AS
      Z(NGRP2,I)=0.0                                                          301AS
      DO 73 N=1,NGR                                                           302AS
      Z(N,I)=0.0                                                              303AS
      P(N,2,I)=0.0                                                            303AS
   73 P(N,3,I)=0.0                                                            304AS
      DO 80 N=1,NGR                                                           315AS
      CALL NORM(N)                                                            320AS
      DO 75 I=1,MAXR                                                          325AS
      Z(N,I)=1.0-P(N,3,I)                                                     330AS
   75 Z(NGRP2,I)=Z(NGRP2,I)+Q(N)*P(N,3,I)                                     335AS
      CALL STORE(N,1)                                                         340AS
   80 CALL STORE(N,2)                                                         345AS
      CALL STORE(NGRP2,2)                                                     350AS
      IF (SENSE SWITCH 1) 81,82                                               351AS
   81 PRINT 1020,                                                             352AS
 1020 FORMAT(105H RESET SENSE SWITCHES AND PRESS START KEY TO GET THE RE      353AS
     1SULTS TO BE CONSTRUCTED FROM INFORMATION ON TAPE 8 ///// )              354AS
      OUTPUT,1025,                                                            355AS
 1025 FORMAT (30H1FORCED EXIT BY SENSE SWITCH 1 ///// )                       356AS
      PAUSE 77777                                                             357AS
      GO TO 87                                                                358AS
   82 DO 85 I=1,MAXR                                                          359AS
      IF (ABSF(Z(NGRP1,I)-Z(NGRP2,I))-ZTEST) 85,85,90                         360AS
   85 CONTINUE                                                                365AS
   87 ENDFILE 8                                                               370AS
      REWIND 8                                                                375AS
      CALL RESULT                                                             380AS
      REWIND 8                                                                384AS
      GO TO 3                                                                 385AS
   90 DO 95 I=1,MAXR                                                          390AS
   95 Z(NGRP1,I)=Z(NGRP2,I)                                                   395AS
      CALL ERASE (Y(1,1),Y(NGRP1,IDIM))                                       400AS
      CALL ERASE (YT(1,1),YT(NGR,IDIM))                                       405AS
      DO 100 N=1,NGRP1                                                        410AS
      CALL CALY(N)                                                            415AS
      IF (N-NGRP1) 100,97,97                                                  416AS
```

```
 97 DO 98 I=2,MAXR                                                                                    417AS
 98 Y(NGRP1,I)=Y(NGRP1,I)*TOTN/Y(NGRP1,1)                                                             418AS
    Y(NGRP1,1)=TOTN                                                                                   419AS
100 CALL STORE(N,3)                                                                                   420AS
    DO 110 N=1,NGR                                                                                    425AS
    DO 105 I=1,MAXR                                                                                   430AS
105 YT(N,I)=Y(NGRP1,I)+Y(N,I)                                                                         435AS
110 CALL STORE(N,4)                                                                                   440AS
    DO 115 N=1,NGR                                                                                    445AS
115 V0(N)=((-3.0)*YT(N,1)+4.0*YT(N,2)-YT(N,3))/(2.0*(R(N,2)-R(N,1)))                                  450AS
120 CALL ERASE (C(1,1),C(NGR,4))                                                                      460AS
    DO 125 N=1,NGR                                                                                    465AS
125 CALL COE (N)                                                                                      470AS
    DO 126 N=1,NGR                                                                                    475AS
    DO 126 I=1,IDIM                                                                                   476AS
126 P(N,1,I)=0.0                                                                                      477AS
    DO 185 N=1,NGR                                                                                    480AS
    DEL=R(N,2)                                                                                        485AS
    D1=YT(N,1)/((R(N,1)-R(N,2))*(R(N,1)-R(N,3)))                                                      490AS
    D2=YT(N,2)/((R(N,2)-R(N,1))*(R(N,2)-R(N,3)))                                                      495AS
    D3=YT(N,3)/((R(N,3)-R(N,1))*(R(N,3)-R(N,2)))                                                      500AS
    R1=R(N,1)                                                                                         505AS
    R2=R(N,2)                                                                                         510AS
    R3=R(N,3)                                                                                         515AS
    CALL ERASE (AGP(1),AGP(35))                                                                       520AS
    CALL ERASE (AGR(1),AGR(35))                                                                       525AS
    CALL ERASE (AGY(1),AGY(35))                                                                       530AS
    AGY(1)=YT(N,1)                                                                                    535AS
    K=0                                                                                               540AS
130 AGR(2)=DEL                                                                                        545AS
    AGR(3)=DEL+DEL                                                                                    550AS
    AGP(2)=0.0                                                                                        555AS
    AGP(3)=0.0                                                                                        560AS
    DO 135 I=1,4                                                                                      565AS
    AGP(2)=AGP(2)+C(N,I)*(AGR(2)**I)                                                                  570AS
135 AGP(3)=AGP(3)+C(N,I)*(AGR(3)**I)                                                                  575AS
    D2P=(E(N)-2.0*YINTF(AGR(2))/AGR(2))*AGP(2)                                                        580AS
```

```
     DEL2P=(AGP(3)-2.0*AGP(2))/(DEL*DEL)                                585AS
     IF (ABSF(D2P-DEL2P)-(TD2P*ABSF(D2P))) 155,155,140                  590AS
140  IF (K-5) 150,145,145                                               595AS
145  CALL ERROR(5,N,K,0)                                                600AS
     GO TO 155                                                          602AS
150  K=K+1                                                              605AS
     DEL=DEL/2.0                                                        610AS
     GO TO 130                                                          615AS
155  IF (K) 165,160,165                                                 620AS
160  IMAX=2                                                             625AS
     GO TO 175                                                          630AS
165  IMAX=2**K+1                                                        635AS
     DO 170 I=2,IMAX                                                    640AS
     AGR(I)=AGR(I-1)+DEL                                                645AS
170  AGY(I)=YINTF(AGR(I))                                               650AS
     CALL INTEG(N,3)                                                    655AS
175  TEST=DEL*0.001                                                     660AS
     IF (ABSF(AGR(IMAX)-R(N,2))-TEST) 185,185,180                       665AS
180  CALL ERROR(6,N,0,0)                                                670AS
     GO TO 87                                                           672AS
185  P(N,1,2)=AGP(IMAX)                                                 675AS
     DO 190 N=1,NGR                                                     680AS
190  CALL INTEG(N,1)                                                    685AS
     CALL ERASE (PRO(1),PRO(NGR))                                       690AS
     DO 225 N=1,NGR                                                     695AS
     IMAX=IRMAX(N)                                                      700AS
     FR=E(N)-2.0*YT(N,IMAX-1)/R(N,IMAX-1)                               705AS
     IF (FR) 195,195,200                                                710AS
195  CALL ERROR(7,N,0,0)                                                715AS
200  DEL=R(N,IMAX)-R(N,IMAX-1)                                          720AS
     TEST=DEL*0.001                                                     725AS
     DNEW=R(N,IMAX-1)-R(N,IMAX-2)                                       730AS
     SQDEL=DEL*DEL                                                      735AS
     IF (ABSF(DEL-DNEW)-TEST) 210,210,205                               740AS
205  CALL ERROR(8,N,0,0)                                                745AS
     GO TO 87                                                           747AS
210  X=0.0                                                              750AS
```

```
      DO 215 K=1,100                                                    755AS
      X1=X                                                              760AS
      X=SQRTF((1.0+X1)*SQDEL*FR)                                        765AS
      IF (ABSF(X-X1)-XTEST) 220,220,215                                 770AS
  215 CONTINUE                                                          775AS
      CALL ERROR(9,N,100,0)                                             780AS
  220 P(N,1,IMAX)=AIN(N)/(1.0+X)                                        785AS
      P(N,1,IMAX-1)=AIN(N)                                              790AS
      P(N,1,IMAX-2)=AIN(N)*(1.0+X)                                      795AS
      CALL INTEG(N,2)                                                   800AS
  225 P(N,1,IMAX)=0.0                                                   805AS
      CALL ERASE (PIN(1),PIN(NGR))                                      810AS
      CALL ERASE (POUT(1),POUT(NGR))                                    815AS
      DO 230 N=1,NGR                                                    820AS
      I=IR0(N)                                                          825AS
      D1=P(N,1,I-2)/((R(N,I-2)-R(N,I-1))*(R(N,I-2)-R(N,I)))             830AS
      D2=P(N,1,I-1)/((R(N,I-1)-R(N,I-2))*(R(N,I-1)-R(N,I)))             835AS
      D3=P(N,1,I)/((R(N,I)-R(N,I-2))*(R(N,I)-R(N,I-1)))                 840AS
      R1=R(N,I-1)+R(N,I)                                                845AS
      R2=R(N,I-2)+R(N,I)                                                850AS
      R3=R(N,I-2)+R(N,I-1)                                              855AS
      A=2.0*(D1+D2+D3)                                                  860AS
      B=-(R1*D1+R2*D2+R3*D3)                                            865AS
      POUT(N)=PRIMEF(R(N,I))/P(N,1,I)                                   870AS
      D1=PR0(N)/((R(N,I)-R(N,I+1))*(R(N,I)-R(N,I+2)))                   875AS
      D2=P(N,1,I+1)/((R(N,I+1)-R(N,I))*(R(N,I+1)-R(N,I+2)))             880AS
      D3=P(N,1,I+2)/((R(N,I+2)-R(N,I))*(R(N,I+2)-R(N,I+1)))             885AS
      R1=R(N,I+1)+R(N,I+2)                                              890AS
      R2=R(N,I)+R(N,I+2)                                                895AS
      R3=R(N,I)+R(N,I+1)                                                900AS
      A=2.0*(D1+D2+D3)                                                  905AS
      B=-(R1*D1+R2*D2+R3*D3)                                            910AS
  230 PIN(N)=PRIMEF(R(N,I))/PR0(N)                                      915AS
      DO 235 N=1,NGR                                                    920AS
      IF (ABSF(PIN(N)-POUT(N))-PTEST) 235,235,238                       925AS
  235 CONTINUE                                                          930AS
      DO 237 N=1,NGR                                                    931AS
```

```
      IMIN=IRO(N)+1                                                          932AS
      IMAX=IRMAX(N)                                                          932AS
      DO 237 I=IMIN,IMAX                                                     933AS
  237 P(N,1,I)=P(N,1,I)*(P(N,1,IMIN-1)/PRO(N))                               934AS
      GO TO 70                                                               935AS
  238 DO 239 N=1,NGR                                                         937AS
      DO 239 I=1,IDIM                                                        938AS
      P(N,2,I)=0.0                                                           939AS
  239 P(N,3,I)=0.0                                                           940AS
      ITE=ITE+1                                                              941AS
      IF (SENSE SWITCH 2) 241,242                                            941AS
  241 PRINT 1020,                                                            942AS
      OUTPUT,1030,                                                           943AS
 1030 FORMAT (30H1FORCED EXIT BY SENSE SWITCH 2 ///// )                      943AS
      PAUSE 77777                                                            943AS
      GO TO 87                                                               944AS
  242 DO 275 N=1,NGR                                                         945AS
      JUMP=IRO(N)                                                            950AS
      IMAX=IRMAX(N)                                                          955AS
      DO 260 I=1,IMAX                                                        960AS
      IF (I-JUMP) 245,250,255                                                965AS
  245 P(N,2,I)=P(N,1,I)/P(N,1,JUMP)                                          970AS
      GO TO 260                                                              975AS
  250 P(N,2,JUMP)=1.0                                                        980AS
      GO TO 260                                                              985AS
  255 P(N,2,I)=P(N,1,I)/PRO(N)                                               990AS
  260 P(N,2,I)=P(N,2,I)*P(N,2,I)                                             995AS
      P(N,3,IMAX)=0.0                                                        997AS
      I=IMAX-1                                                              1000AS
  265 P(N,3,I)=(P(N,2,I)+P(N,2,I+1))*(R(N,I+1)-R(N,I))/2.0+P(N,3,I+1)       1005AS
      IF (I-1) 275,275,270                                                  1010AS
  270 I=I-1                                                                 1015AS
      GO TO 265                                                             1020AS
  275 E(N)=E(N)-(POUT(N)-PIN(N))/P(N,3,1)                                   1025AS
      IF (SENSE SWITCH 6) 280,120                                           1026AS
  280 PRINT 1035,ITE                                                        1027AS
 1035 FORMAT (31H BEGINNING CYCLE WITH E NUMBER I3 ///// )                  1028AS
```

```
      GO TO 120                                                          1030AS
      END                                                                1035AS
*     CARDS COLUMN
      SUBROUTINE SETUP (N)                                                5SE
      DIMENSION AGP(35),AGR(35),AGY(35),AIN(2),AOUT(2),C(2,4),E(2),IRMAX    10AS
     1(2),IRO(2),ITER(10),OUT(10,150),P(2,3,150),PIN(2),POUT(2),PRO(2),Q    15AS
     2(2),R(2,150),V0(2),Y(3,150),YT(2,150),Z(4,150)                        20AS
      COMMON AGP,AGR,AGY,AIN,AOUT,C,E,IRMAX,IRO,ITER,OUT,P,PIN,POUT,PRO,    25AS
     1Q,R,V0,Y,YT,Z,ALPHA,D1,D2,D3,D2P,DEL,DEL2P,DNEW,FR,IDIM,IMAX,IMIN,    30AS
     2ITE,ITP,JUMP,K1,K2,K3,KMAX,KMIN,MAXR,NAME1,NAME2,NGR,NGRP1,NGRP2,     35AS
     3PI,PIM2,PIP2,PTEST,R1,R2,R3,SQDEL,SQN,TD2P,TEST,TNORM,TOTN,X1,        40AS
     4XTEST,ZTEST,A,B,X                                                     45AS
      INPUT,1100,NCODE                                                    10SE
 1100 FORMAT (I2)                                                         15SE
      IF (N-NCODE) 5,10,5                                                 20SE
    5 CALL ERROR (10,N,0,0)                                               25SE
   10 INPUT,1105,IRMAX(N),IRO(N),E(N),Q(N),AIN(N)                         30SE
 1105 FORMAT (2X,2I4,3F10.5)                                             35SE
      MA=IRMAX(N)                                                        40SE
      INPUT,1110,(R(N,I),I=1,MA)                                         45SE
 1110 FORMAT (2X,F8.4,8X,F8.4,8X,F8.4,8X,F8.4)                           50SE
      GO TO (15,25),N                                                    55SE
   15 DO 20 I=1,MA                                                       60SE
   20 P(N,1,I)=16.0*R(N,I)*EXPF(-4.0*R(N,I))                             65SE
      GO TO 35                                                           70SE
   25 A=16.0/SQRTF(2.0)                                                  75SE
      DO 30 I=1,MA                                                       80SE
   30 P(N,1,I)=A*R(N,I)*(0.5-R(N,I))*EXPF(-2.0*R(N,I))                   85SE
   35 P(N,1,MA)=0.0                                                     100SE
      RETURN                                                            105SE
      END                                                               110SE
*     CARDS COLUMN
      SUBROUTINE NORM (N)                                                 5NO
      DIMENSION AGP(35),AGR(35),AGY(35),AIN(2),AOUT(2),C(2,4),E(2),IRMAX    10AS
     1(2),IRO(2),ITER(10),OUT(10,150),P(2,3,150),PIN(2),POUT(2),PRO(2),Q    15AS
     2(2),R(2,150),V0(2),Y(3,150),YT(2,150),Z(4,150)                        20AS
      COMMON AGP,AGR,AGY,AIN,AOUT,C,E,IRMAX,IRO,ITER,OUT,P,PIN,POUT,PRO,    25AS
```

```
     1Q,R,V0,Y,YT,Z,ALPHA,D1,D2,D3,D2P,DEL,DEL2P,DNEW,FR,IDIM,IMAX,IMIN,     30AS
     2ITE,ITP,JUMP,K1,K2,K3,KMAX,KMIN,MAXR,NAME1,NAME2,NGR,NGRP1,NGRP2,     35AS
     3PI,PIM2,PIP2,PTEST,R1,R2,R3,SQDEL,SQN,TD2P,TEST,TNORM,TOTN,X1,        40AS
     4XTEST,ZTEST,A,B,X                                                     45AS
      IMAX=IRMAX(N)                                                         10NO
      IMAXM1=IMAX-1                                                         15NO
      DO 5 I=1,IMAX                                                         20NO
   5  P(N,2,I)=P(N,1,I)*P(N,1,I)                                            25NO
      P(N,3,IMAX)=0.0                                                       30NO
      DO 10 I=1,IMAXM1                                                      35NO
      K=IMAX-I                                                              40NO
      KP1=K+1                                                               45NO
  10  P(N,3,K)=P(N,3,KP1)+((R(N,KP1)-R(N,K))/2.0)*(P(N,2,K)+P(N,2,KP1))     50NO
      IF (ABSF(P(N,3,1)-1.0)-TNORM) 30,15,15                                55NO
  15  X=SQRTF(P(N,3,1))                                                     57NO
      DO 20 I=1,IMAX                                                        60NO
      P(N,1,I)=P(N,1,I)/X                                                   65NO
  20  P(N,2,I)=P(N,1,I)*P(N,1,I)                                            70NO
      DO 25 I=2,IMAX                                                        75NO
  25  P(N,3,I)=P(N,3,I)/P(N,3,1)                                            80NO
      P(N,3,1)=1.0                                                          85NO
  30  AOUT(N)=ABSF(P(N,1,1))                                                90NO
      DO 40 I=2,IMAX                                                        95NO
      TEST=ABSF(P(N,1,I))                                                  100NO
      IF (AOUT(N)-TEST) 35,40,40                                           105NO
  35  AOUT(N)=TEST                                                         110NO
  40  CONTINUE                                                             115NO
      AOUT(N)=ALPHA/AOUT(N)                                                120NO
      RETURN                                                               125NO
      END                                                                  130NO
*     CARDS COLUMN
      SUBROUTINE COE  (N)                                                    5CO
      DIMENSION AGP(35),AGR(35),AGY(35),AIN(2),AOUT(2),C(2,4),E(2),IRMAX     10AS
     1(2),IRO(2),ITER(10),OUT(10,150),P(2,3,150),PIN(2),POUT(2),PRO(2),Q     15AS
     2(2),R(2,150),V0(2),Y(3,150),YT(2,150),Z(4,150)                         20AS
      COMMON AGP,AGR,AGY,AIN,AOUT,C,E,IRMAX,IRO,ITER,OUT,P,PIN,POUT,PRO,     25AS
     1Q,R,V0,Y,YT,Z,ALPHA,D1,D2,D3,D2P,DEL,DEL2P,DNEW,FR,IDIM,IMAX,IMIN,     30AS
```

```
     2ITE,ITP,JUMP,K1,K2,K3,KMAX,KMIN,MAXR,NAME1,NAME2,NGR,NGRP1,NGRP2,      35AS
     3PI,PIM2,PIP2,PTEST,R1,R2,R3,SQDEL,SQN,TD2P,TEST,TNORM,TOTN,X1,         40AS
     4XTEST,ZTEST,A,B,X                                                      45AS
      C(N,1)=AOUT(N)                                                         10CO
      C(N,2)=-AOUT(N)*TOTN                                                   15CO
      VME=2.0*V0(N)-E(N)                                                     20CO
      C(N,3)=AOUT(N)*(2.0*SQN-VME)/6.0                                       25CO
      C(N,4)=AOUT(N)*(-TOTN/18.0)*(SQN-2.0*VME)                              30CO
      RETURN                                                                 35CO
      END                                                                    40CO
*     CARDS COLUMN
      SUBROUTINE CALY (N)                                                     5CA
      DIMENSION AGP(35),AGR(35),AGY(35),AIN(2),AOUT(2),C(2,4),E(2),IRMAX     10AS
     1(2),IR0(2),ITER(10),OUT(10,150),P(2,3,150),PIN(2),POUT(2),PR0(2),Q     15AS
     2(2),R(2,150),V0(2),Y(3,150),YT(2,150),Z(4,150)                         20AS
      COMMON AGP,AGR,AGY,AIN,AOUT,C,E,IRMAX,IR0,ITER,OUT,P,PIN,POUT,PR0,     25AS
     1Q,R,V0,Y,YT,Z,ALPHA,D1,D2,D3,D2P,DEL,DEL2P,DNEW,FR,IDIM,IMAX,IMIN,     30AS
     2ITE,ITP,JUMP,K1,K2,K3,KMAX,KMIN,MAXR,NAME1,NAME2,NGR,NGRP1,NGRP2,      35AS
     3PI,PIM2,PIP2,PTEST,R1,R2,R3,SQDEL,SQN,TD2P,TEST,TNORM,TOTN,X1,         40AS
     4XTEST,ZTEST,A,B,X                                                      45AS
      IMAX=MAXR-1                                                            10CA
      DO 5 I=1,IMAX                                                          15CA
      K=MAXR-I                                                               20CA
      KP1=K+1                                                                25CA
    5 Y(N,K)=(R(N,K)*Y(N,KP1)+(R(N,KP1)-R(N,K))*Z(N,K   ))/R(N,KP1)          30CA
      RETURN                                                                 35CA
      END                                                                    40CA
*     CARDS COLUMN
      SUBROUTINE INTEG (N,K)                                                  5IN
      DIMENSION AGP(35),AGR(35),AGY(35),AIN(2),AOUT(2),C(2,4),E(2),IRMAX     10AS
     1(2),IR0(2),ITER(10),OUT(10,150),P(2,3,150),PIN(2),POUT(2),PR0(2),Q     15AS
     2(2),R(2,150),V0(2),Y(3,150),YT(2,150),Z(4,150)                         20AS
      COMMON AGP,AGR,AGY,AIN,AOUT,C,E,IRMAX,IR0,ITER,OUT,P,PIN,POUT,PR0,     25AS
     1Q,R,V0,Y,YT,Z,ALPHA,D1,D2,D3,D2P,DEL,DEL2P,DNEW,FR,IDIM,IMAX,IMIN,     30AS
     2ITE,ITP,JUMP,K1,K2,K3,KMAX,KMIN,MAXR,NAME1,NAME2,NGR,NGRP1,NGRP2,      35AS
     3PI,PIM2,PIP2,PTEST,R1,R2,R3,SQDEL,SQN,TD2P,TEST,TNORM,TOTN,X1,         40AS
     4XTEST,ZTEST,A,B,X                                                      45AS
```

```
      PINTF(X)=(X-R2)*(X-R3)*D1+(X-R1)*(X-R3)*D2+(X-R1)*(X-R2)*D3          10IN
      GO TO (5,50,110),K                                                   15IN
    5 IMAX=IR0(N)                                                          20IN
      DEL=R(N,2)-R(N,1)                                                    25IN
      SQDEL=DEL*DEL                                                        30IN
      TEST=DEL*0.001                                                       35IN
      DO 45 I=3,IMAX                                                       40IN
      DNEW=R(N,I)-R(N,I-1)                                                 45IN
      IF (ABSF(DEL-DNEW)-TEST) 10,10,15                                    50IN
   10 PIM2=P(N,1,I-2)                                                      55IN
      GO TO 45                                                             60IN
   15 K3=I-1                                                               65IN
      K1=I-3                                                               70IN
   20 IF (K1) 25,25,30                                                     75IN
   25 CALL ERROR (11,N,0,0)                                                80IN
   30 IF ((R(N,K3)-R(N,K1))-DNEW) 35,40,40                                 85IN
   35 K1=K1-1                                                              90IN
      GO TO 20                                                             95IN
   40 K2=K1+1                                                             100IN
      D1=P(N,1,K1)/((R(N,K1)-R(N,K2))*(R(N,K1)-R(N,K3)))                  105IN
      D2=P(N,1,K2)/((R(N,K2)-R(N,K1))*(R(N,K2)-R(N,K3)))                  110IN
      D3=P(N,1,K3)/((R(N,K3)-R(N,K1))*(R(N,K3)-R(N,K2)))                  115IN
      R1=R(N,K1)                                                          120IN
      R2=R(N,K2)                                                          125IN
      R3=R(N,K3)                                                          130IN
      DEL=DNEW                                                            135IN
      SQDEL=DEL*DEL                                                       140IN
      TEST=DEL*0.001                                                      145IN
      PIM2=PINTF(R(N,I-1)-DEL)                                            150IN
   45 P(N,1,I)=((E(N)-2.0*YT(N,I-1)/R(N,I-1))*SQDEL+2.0)*P(N,1,I-1)-PIM2  155IN
      GO TO 120                                                           160IN
   50 IMIN=IR0(N)                                                         165IN
      IMAX=IRMAX(N)                                                       170IN
      DEL=R(N,IMAX)-R(N,IMAX-1)                                           175IN
      SQDEL=DEL*DEL                                                       180IN
      TEST=DEL*0.001                                                      185IN
      I=IMAX-3                                                            190IN
```

```
   55 DNEW=R(N,I+1)-R(N,I)                                                    195IN
      IF (ABSF(DEL-DNEW)-TEST) 60,60,65                                       200IN
   60 PIP2=P(N,1,I+2)                                                         205IN
      GO TO 95                                                                210IN
   65 K3=I+3                                                                  215IN
      K1=I+1                                                                  220IN
   70 IF (K3-IMAX) 80,80,75                                                   225IN
   75 CALL ERROR (12,N,0,0)                                                   230IN
   80 IF ((R(N,K3)-R(N,K1))-DNEW) 85,90,90                                    235IN
   85 K3=K3+1                                                                 240IN
      GO TO 70                                                                245IN
   90 K2=K3-1                                                                 250IN
      D1=P(N,1,K1)/((R(N,K1)-R(N,K2))*(R(N,K1)-R(N,K3)))                      255IN
      D2=P(N,1,K2)/((R(N,K2)-R(N,K1))*(R(N,K2)-R(N,K3)))                      260IN
      D3=P(N,1,K3)/((R(N,K3)-R(N,K1))*(R(N,K3)-R(N,K2)))                      265IN
      R1=R(N,K1)                                                              270IN
      R2=R(N,K2)                                                              275IN
      R3=R(N,K3)                                                              280IN
      DEL=DNEW                                                                285IN
      SQDEL=DEL*DEL                                                           290IN
      TEST=DEL*0.001                                                          295IN
      PIP2=PINTF(R(N,I+1)+DEL)                                                300IN
   95 PI=((E(N)-2.0*YT(N,I+1)/R(N,I+1))*SQDEL+2.0)*P(N,1,I+1)-PIP2            305IN
      IF (I-IMIN) 105,105,100                                                 310IN
  100 P(N,1,I)=PI                                                             315IN
      I=I-1                                                                   320IN
      GO TO 55                                                                325IN
  105 PRO(N)=PI                                                               330IN
      GO TO 120                                                               335IN
  110 SQDEL=DEL*DEL                                                           340IN
      DO 115 I=3,IMAX                                                         345IN
  115 AGP(I)=((E(N)-2.0*AGY(I-1)/AGR(I-1))*SQDEL+2.0)*AGP(I-1)-AGP(I-2)       350IN
  120 CONTINUE                                                                355IN
      RETURN                                                                  360IN
      END                                                                     365IN
*     CARDS COLUMN
      SUBROUTINE STORE (N,K)                                                   5ST
```

```
      DIMENSION AGP(35),AGR(35),AGY(35),AIN(2),AOUT(2),C(2,4),E(2),IRMAX     10AS
     1(2),IR0(2),ITER(10),OUT(10,150),P(2,3,150),PIN(2),POUT(2),PR0(2),Q     15AS
     2(2),R(2,150),V0(2),Y(3,150),YT(2,150),Z(4,150)                         20AS
      COMMON AGP,AGR,AGY,AIN,AOUT,C,E,IRMAX,IR0,ITER,OUT,P,PIN,POUT,PR0,     25AS
     1Q,R,V0,Y,YT,Z,ALPHA,D1,D2,D3,D2P,DEL,DEL2P,DNEW,FR,IDIM,IMAX,IMIN,     30AS
     2ITE,ITP,JUMP,K1,K2,K3,KMAX,KMIN,MAXR,NAME1,NAME2,NGR,NGRP1,NGRP2,     35AS
     3PI,PIM2,PIP2,PTEST,R1,R2,R3,SQDEL,SQN,TD2P,TEST,TNORM,TOTN,X1,        40AS
     4XTEST,ZTEST,A,B,X                                                      45AS
      WRITE OUTPUT TAPE 8,1300,N,K                                           10ST
 1300 FORMAT (I2,I1)                                                         15ST
      GO TO (5,10,15,20),K                                                   20ST
    5 WRITE OUTPUT TAPE 8,1305,(P(N,1,I),I=1,MAXR)                          25ST
 1305 FORMAT (3X,10F10.5)                                                    30ST
      GO TO 25                                                               35ST
   10 WRITE OUTPUT TAPE 8,1305,(Z(N,I),I=1,MAXR)                            40ST
      GO TO 25                                                               45ST
   15 WRITE OUTPUT TAPE 8,1305,(Y(N,I),I=1,MAXR)                            50ST
      GO TO 25                                                               55ST
   20 WRITE OUTPUT TAPE 8,1305,(YT(N,I),I=1,MAXR)                           60ST
   25 CONTINUE                                                              65ST
      RETURN                                                                70ST
      END                                                                   75ST
*     CARDS COLUMN
      SUBROUTINE ERROR (J,N,M,I)                                             5ER
      DIMENSION AGP(35),AGR(35),AGY(35),AIN(2),AOUT(2),C(2,4),E(2),IRMAX     10AS
     1(2),IR0(2),ITER(10),OUT(10,150),P(2,3,150),PIN(2),POUT(2),PR0(2),Q     15AS
     2(2),R(2,150),V0(2),Y(3,150),YT(2,150),Z(4,150)                         20AS
      COMMON AGP,AGR,AGY,AIN,AOUT,C,E,IRMAX,IR0,ITER,OUT,P,PIN,POUT,PR0,     25AS
     1Q,R,V0,Y,YT,Z,ALPHA,D1,D2,D3,D2P,DEL,DEL2P,DNEW,FR,IDIM,IMAX,IMIN,     30AS
     2ITE,ITP,JUMP,K1,K2,K3,KMAX,KMIN,MAXR,NAME1,NAME2,NGR,NGRP1,NGRP2,     35AS
     3PI,PIM2,PIP2,PTEST,R1,R2,R3,SQDEL,SQN,TD2P,TEST,TNORM,TOTN,X1,        40AS
     4XTEST,ZTEST,A,B,X                                                      45AS
      OUTPUT,1200,J,ITP,ITE                                                  10ER
 1200 FORMAT (15H1ERROR OF TYPE I3,21H OCCURRED DURING THE I3,28H -TH IT     15ER
     1ERATION ON P AND THE I3,20H -TH ITERATION ON E. ///)                   20ER
      GO TO (5,10,15,15,20,25,30,35,40,45,50,55),J                           25ER
    5 OUTPUT,1205,MAXR                                                       30ER
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1205 FORMAT (22H ERROR IN CALCULATING I3 ///)                                    35ER
     GO TO 60                                                                   40ER
  10 OUTPUT,1210,N,I,R(N,I),M,I,R(M,I)                                          45ER
1210 FORMAT (21H R-S DO NOT MATCH (R( I2,2H , I3,3H )= E13.6,10H     AND       50ER
    1 R( I2,2H , I3,3H )= E13.6,22H ).  CORRECT AND RERUN ///)                  55ER
     GO TO 60                                                                   60ER
  15 OUTPUT,1215,N,N,P(N,1,IMAX)                                                65ER
1215 FORMAT (36H P(NL,R) IS NOT ZERO AT INFINITE, P( I2,10H ,1,IRMAX( I         70ER
    I2, 4H ))= E13.6,36H .  MAKE CHANGES NECESSARY AND RERUN ///)               75ER
     GO TO 60                                                                   80ER
  20 OUTPUT,1220,N,D2P,DEL2P,M,DEL                                              85ER
1220 FORMAT (14H FOR NL-GROUP I2,85H THE TAYLOR SERIES EXPANSION DOES N         90ER
    1OT GIVE AGREEMENT BETWEEN SECOND DERIVATIVE, D2P= E13.6, // 33H ,          95ER
    2AND SECOND DIFFERENCE, DEL2P= E13.6, 9H , AFTER I2,27H SUBDIVISION        100ER
    3S SO THAT DEL= E13.6 ///)                                                 105ER
     GO TO 60                                                                  110ER
  25 OUTPUT,1225,IMAX,AGR(IMAX),N,R(N,2),TEST                                  115ER
1225 FORMAT ( 5H AGR( I3,4H )= E13.6, 6H ,  R( I2, 6H ,2)= E13.6,22H FA        120ER
    1ILED TO MEET TEST= E13.6 ///)                                             125ER
     GO TO 60                                                                  130ER
  30 OUTPUT,1230,N,FR                                                          135ER
1230 FORMAT (14H FOR NL-GROUP I2, 9H , F(R)= E13.6,30H , BUT SHOULD BE         140ER
    1NON-NEGATIVE, ///)                                                        145ER
     GO TO 60                                                                  150ER
  35 OUTPUT,1235,N                                                             155ER
1235 FORMAT (85H INTEGRATION SCHEME REQUIRES THAT THE LAST THRE R-S BE         160ER
    1EQUALLY SPACED.  FOR NL-GROUP I2,28H THIS REQUIREMENT IS NOT MET/)        165ER
     GO TO 60                                                                  170ER
  40 OUTPUT,1240,N,M,XTEST,X1                                                  175ER
1240 FORMAT (14H FOR NL-GROUP I2,95H , THE ITERATION SCHEME FOR FINDING        180ER
    1 X TO INITIALIZE INWARD INTEGRATION HAS NOT CONVERGED AFTER // I5,        185ER
    230H ITERATIONS, TO WITHIN XTEST= E13.6,21H .  AT THAT POINT X1=E13        190ER
    3.6//56H  IF NO MISTAKES WERE MADE, THE PROGRAM MUST BE MODIFIED//)        195ER
     GO TO 60                                                                  200ER
  45 OUTPUT,1245,N                                                             205ER
1245 FORMAT (72H PROGRAMMER DOES NOT KNOW HOW TO STACK INPUT DATA.  MIS        210ER
    1TAKE AT NL-GROUP I2 ///)                                                  215ER
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      CALL EXIT                                                          220ER
   50 OUTPUT,1250,N                                                      225ER
 1250 FORMAT (84H IN CHANGING INCREMENT LENGTHS, THE INTERPOLATION SCHEM  230ER
     1E DECREASED A SUBSCRIPT TO 0. // 55H THIS OCCURRED DURING OUTWARD   235ER
     2INTEGRATION FOR NL-GROUP I2 ///)                                   240ER
      GO TO 57                                                           245ER
   55 OUTPUT,1255,                                                       250ER
 1255 FORMAT (96H IN CHANGING INCREMENT LENGTHS, THE INTERPOLATION SCHEM  255ER
     1E INCREASED A SUBSCRIPT BEYOND ITS RANGE. // 54H THIS OCCURRED DUR  260ER
     2ING INWARD INTEGRATION FOR NL-GROUP I2 ///)                        265ER
   57 CALL RESULT                                                        270ER
      CALL EXIT                                                          275ER
   60 CONTINUE                                                           280ER
      RETURN                                                             285ER
      END                                                                290ER
*     CARDS COLUMN
      SUBROUTINE RESULT                                                    5RE
      DIMENSION AGP(35),AGR(35),AGY(35),AIN(2),AOUT(2),C(2,4),E(2),IRMAX   10AS
     1(2),IR0(2),ITER(10),OUT(10,150),P(2,3,150),PIN(2),POUT(2),PR0(2),Q   15AS
     2(2),R(2,150),V0(2),Y(3,150),YT(2,150),Z(4,150)                       20AS
      COMMON AGP,AGR,AGY,AIN,AOUT,C,E,IRMAX,IR0,ITER,OUT,P,PIN,POUT,PR0,   25AS
     1Q,R,V0,Y,YT,Z,ALPHA,D1,D2,D3,D2P,DEL,DEL2P,DNEW,FR,IDIM,IMAX,IMIN,   30AS
     2ITE,ITP,JUMP,K1,K2,K3,KMAX,KMIN,MAXR,NAME1,NAME2,NGR,NGRP1,NGRP2,   35AS
     3PI,PIM2,PIP2,PTEST,R1,R2,R3,SQDEL,SQN,TD2P,TEST,TNORM,TOTN,X1,      40AS
     4XTEST,ZTEST,A,B,X                                                    45AS
      OUTPUT,1400,NAME1,NAME2,ITP,ITE                                      10RE
 1400 FORMAT (22H1ATOMIC STRUCTURE FOR 2A6, //// 7H AFTER I3,27H ITERATI   15RE
     1ONS ON THE P-S AND I3, 22H ITERATIONS ON THE E-S // 46H THE CALCUL    20RE
     2ATED   E-S    FOR THE NL-GROUPS ARE ////)                           25RE
      DO 5 N=1,NGR                                                         30RE
    5 OUTPUT,1405,N,E(N)                                                   35RE
 1405 FORMAT ( 3H0E( I2, 4H )= E13.6)                                      40RE
      DO 130 N=1,NGRP2                                                     45RE
      IF (N-NGRP1) 10,12,15                                                50RE
   10 KMIN=1                                                               55RE
      KMAX=4                                                               60RE
      GO TO 20                                                             65RE
```

```
   12 KMIN=3                                                                    66RE
      KMAX=3                                                                    67RE
      GO TO 20                                                                  68RE
   15 KMIN=2                                                                    70RE
      KMAX=2                                                                    75RE
   20 DO 130 K=KMIN,KMAX                                                        80RE
      K1=10*N+K                                                                 85RE
      K3=1                                                                      90RE
   25 CALL ERASE (OUT(1,1),OUT(10,IDIM))                                        95RE
      J=1                                                                      100RE
   30 IF (EOF(8)) 35,40,35                                                     105RE
   35 M=J-1                                                                    110RE
      IF (M-0) 130,130,70                                                      115RE
   40 READ INPUT TAPE 8,1410,K2                                                120RE
 1410 FORMAT (I3)                                                              125RE
      IF (K2) 45,30,50                                                         130RE
   45 OUTPUT,1415,K2                                                           135RE
 1415 FORMAT ( 8HO ERROR I6,50H IN COLUMNS 1-3 OF TAPE 8, SHOULD NOT BE       140RE
     1NEGATIVE.//// )                                                         145RE
      GO TO 135                                                               150RE
   50 IF (K2-K1) 30,55,30                                                     155RE
   55 READ INPUT TAPE 8,1420,(OUT(J,I),I=1,MAXR)                              160RE
 1420 FORMAT (3X,10F10.5  )                                                   165RE
      ITER(J)=K3                                                              170RE
      K3=K3+1                                                                 172RE
      IF (J-5)  60,65,65                                                      175RE
   60 J=J+1                                                                   180RE
      GO TO 30                                                                190RE
   65 M=5                                                                     195RE
   70 OUTPUT,1425,                                                            200RE
 1425 FORMAT (1H1)                                                            205RE
      GO TO (75,80,95,110),K                                                  210RE
   75 OUTPUT,1430,N                                                          215RE
 1430 FORMAT (14H FOR NL-GROUP I2,29H , THE P(NL,R) ARE AS FOLLOWS ///)       220RE
      GO TO 115                                                               225RE
   80 IF (N-NGR) 85,85,90                                                     230RE
   85 OUTPUT,1435,N                                                          235RE
```

```
 1435 FORMAT (14H FOR NL-GROUP I2,33H , THE Z0(NL,NL,R) ARE AS FOLLOWS /    240RE
     1///)                                                                  245RE
      GO TO 115                                                             250RE
   90 OUTPUT,1440,                                                          255RE
 1440 FORMAT (24H THE Z(R) ARE AS FOLLOWS ///)                              260RE
      GO TO 115                                                             265RE
   95 IF (N-NGR) 100,100,105                                                270RE
  100 OUTPUT,1445,N                                                         275RE
 1445 FORMAT (14H FOR NL-GROUP I2,33H , THE Y0(NL,NL,R) ARE AS FOLLOWS /    280RE
     1///)                                                                  285RE
      GO TO 115                                                             290RE
  105 OUTPUT,1450,                                                          295RE
 1450 FORMAT (24H THE Y(R) ARE AS FOLLOWS ///)                              300RE
      GO TO 115                                                             305RE
  110 OUTPUT,1455,N                                                         310RE
 1455 FORMAT (14H FOR NL-GROUP I2,29H , THE Y(NL,R) ARE AS FOLLOWS ///)     315RE
  115 OUTPUT,1460,(ITER(I),I=1,M)                                           320RE
 1460 FORMAT (11H ITERATION=  9(I3,8X),I3)                                  325RE
      OUTPUT,1465,                                                          330RE
 1465 FORMAT ( 3H0 R // )                                                   335RE
      KLUG=7                                                                340RE
      DO 125 I=1,MAXR                                                       345RE
      OUTPUT,1470,R(N,I),(OUT(J,I),J=1,M)                                   350RE
 1470 FORMAT (F7.2,2X,10(F9.4,2X))                                          355RE
      KLUG=KLUG+1                                                           360RE
      IF (KLUG-60) 125,120,120                                              365RE
  120 OUTPUT,1425,                                                          370RE
      KLUG=0                                                                375RE
  125 CONTINUE                                                              380RE
      GO TO 25                                                              385RE
  130 REWIND 8                                                              390RE
  135 CONTINUE                                                              395RE
      RETURN                                                                435RE
      END                                                                   440RE
*     DATA
 BERYLLIUM     2150 2.0      0.01     0.0001   0.01     0.001    0.01        DATA
 1                                                                        1BERY1
```

```
    36  12    9.4660      2.0        0.0007                                    2BERY1
    0.00      0.000     0.02      0.369     0.04      0.682     0.06      0.946  3BERY1
    0.08      1.166     0.10      1.347     0.12      1.496     0.14      1.615  4BERY1
    0.16      1.709     0.18      1.781     0.20      1.834     0.25      1.898  5BERY1
    0.30      1.889     0.35      1.831     0.40      1.742     0.45      1.633  6BERY1
    0.50      1.515     0.55      1.392     0.60      1.270     0.7       1.038  7BERY1
    0.8       0.834     0.9       0.661     1.0       0.518     1.1       0.403  8BERY1
    1.2       0.311     1.3       0.239     1.4       0.183     1.6       0.105  9BERY1
    1.8       0.060     2.0       0.034     2.2       0.019     2.4       0.011  10BERY1
    2.6       0.006     2.8       0.003     3.0       0.001     3.2       0.000  11BERY1
2                                                                               1BERY2
    52  30    0.6186      2.0       -0.0001                                     2BERY2
    0.00      0.000     0.02      0.369     0.04      0.681     0.06      0.941  3BERY2
    0.08      1.156     0.10      1.329     0.12      1.466     0.14      1.570  4BERY2
    0.16      1.645     0.18      1.694     0.20      1.719     0.25      1.698  5BERY2
    0.30      1.580     0.35      1.391     0.40      1.150     0.45      0.873  6BERY2
    0.50      0.572     0.55      0.256     0.60     -0.068     0.7      -0.717  7BERY2
    0.8      -1.343     0.9      -1.926     1.0      -2.454     1.1      -2.922  8BERY2
    1.2      -3.328     1.3      -3.674     1.4      -3.962     1.6      -4.379  9BERY2
    1.8      -4.615     2.0      -4.704     2.2      -4.680     2.4      -4.571  10BERY2
    2.6      -4.401     2.8      -4.189     3.0      -3.950     3.2      -3.695  11BERY2
    3.4      -3.434     3.6      -3.174     3.8      -2.919     4.0      -2.674  12BERY2
    4.5      -2.112     5.0      -1.639     5.5      -1.254     6.0      -0.949  13BERY2
    7.0      -0.529     8.0      -0.287     9.0      -0.152    10.0      -0.079  14BERY2
   12.0      -0.021    14.0      -0.005    16.0      -0.001    18.0       0.000  15BERY2
BERYLLIUM     2150 2.0          0.01      0.0001    0.01      0.001     0.01     DATA
1                                                                               1BERY1
    36  12    8.0000      2.0        0.0007                                    2BERY1
    0.00      0.000     0.02      0.369     0.04      0.682     0.06      0.946  3BERY1
    0.08      1.166     0.10      1.347     0.12      1.496     0.14      1.615  4BERY1
    0.16      1.709     0.18      1.781     0.20      1.834     0.25      1.898  5BERY1
    0.30      1.889     0.35      1.831     0.40      1.742     0.45      1.633  6BERY1
    0.50      1.515     0.55      1.392     0.60      1.270     0.7       1.038  7BERY1
    0.8       0.834     0.9       0.661     1.0       0.518     1.1       0.403  8BERY1
    1.2       0.311     1.3       0.239     1.4       0.183     1.6       0.105  9BERY1
    1.8       0.060     2.0       0.034     2.2       0.019     2.4       0.011  10BERY1
    2.6       0.006     2.8       0.003     3.0       0.001     3.2       0.000  11BERY1
```

```
2                                                                                  1BERY2
   52  30    0.2000       2.0       -0.0001                                        2BERY2
   0.00      0.000   0.02      0.369   0.04      0.681   0.06      0.941           3BERY2
   0.08      1.156   0.10      1.329   0.12      1.466   0.14      1.570           4BERY2
   0.16      1.645   0.18      1.694   0.20      1.719   0.25      1.698           5BERY2
   0.30      1.580   0.35      1.391   0.40      1.150   0.45      0.873           6BERY2
   0.50      0.572   0.55      0.256   0.60     -0.068   0.7      -0.717           7BERY2
   0.8      -1.343   0.9      -1.926   1.0      -2.454   1.1      -2.922           8BERY2
   1.2      -3.328   1.3      -3.674   1.4      -3.962   1.6      -4.379           9BERY2
   1.8      -4.615   2.0      -4.704   2.2      -4.680   2.4      -4.571          10BERY2
   2.6      -4.401   2.8      -4.189   3.0      -3.950   3.2      -3.695          11BERY2
   3.4      -3.434   3.6      -3.174   3.8      -2.919   4.0      -2.674          12BERY2
   4.5      -2.112   5.0      -1.639   5.5      -1.254   6.0      -0.949          13BERY2
   7.0      -0.529   8.0      -0.287   9.0      -0.152  10.0      -0.079          14BERY2
  12.0      -0.021  14.0      -0.005  16.0      -0.001  18.0       0.000          15BERY2
```

CALCULATION OF ATOMIC STRUCTURE CONATSER

INPUT FOR NEXT CALCULATIONS WERE

ATOM = BERYLLIUM

NGR = 2

IDIM =150

ALPHA = 2.000000

ZTEST = 0.010000

TNORM = 0.000100

TD2P = 0.010000

XTEST = 0.001000

PTEST = 0.010000

IRMAX(1)= 36

IRO(1)= 12

Q(1)= 2.0000

AIN(1)= 0.000700

IRMAX(2)= 52

IRO(2)= 30

Q(2)= 2.0000

```
AIN(  2)= -0.000100
E( 1 )=  0.946600E 01
E( 2 )=  0.618600E 00
```

ATOMIC STRUCTURE FOR BERYLLIUM

AFTER 6 ITERATIONS ON THE P-S AND 11 ITERATIONS ON THE E-S

THE CALCULATED E-S FOR THE NL-GROUPS ARE

E(1)= 0.974711E 01

E(2)= 0.490891E-00

FOR NL-GROUP 1 , THE P(NL,R) ARE AS FOLLOWS

ITERATION=	1	2	3	4	5
R					
0.	0.	0.	0.	0.	0.
0.02	0.2952	0.2717	0.2777	0.2764	0.2767
0.04	0.5449	0.5018	0.5129	0.5104	0.5110
0.06	0.7546	0.6952	0.7104	0.7070	0.7080
0.08	0.9287	0.8564	0.8749	0.8708	0.8719
0.10	1.0717	0.9892	1.0103	1.0055	1.0068
0.12	1.1871	1.0972	1.1201	1.1149	1.1163
0.14	1.2785	1.1835	1.2074	1.2020	1.2035
0.16	1.3488	1.2506	1.2752	1.2696	1.2712
0.18	1.4007	1.3011	1.3258	1.3202	1.3218
0.20	1.4367	1.3371	1.3615	1.3560	1.3575
0.25	1.4703	1.3813	1.4029	1.3980	1.3993
0.30	1.4446	1.3755	1.3924	1.3885	1.3896
0.35	1.3798	1.3350	1.3462	1.3437	1.3444
0.40	1.2911	1.2716	1.2770	1.2759	1.2762
0.45	1.1892	1.1942	1.1940	1.1942	1.1942
0.50	1.0818	1.1090	1.1038	1.1051	1.1048
0.55	0.9743	1.0205	1.0109	1.0133	1.0127
0.60	0.8702	0.9318	0.9188	0.9219	0.9211
0.70	0.6805	0.7648	0.7465	0.7509	0.7497
0.80	0.5213	0.6175	0.5962	0.6012	0.5998
0.90	0.3931	0.4925	0.4700	0.4752	0.4738
1.00	0.2928	0.3893	0.3668	0.3718	0.3705
1.10	0.2159	0.3055	0.2840	0.2887	0.2874
1.20	0.1579	0.2385	0.2185	0.2227	0.2216
1.30	0.1146	0.1855	0.1673	0.1711	0.1700
1.40	0.0828	0.1439	0.1277	0.1310	0.1301
1.60	0.0425	0.0854	0.0730	0.0754	0.0747
1.80	0.0215	0.0502	0.0413	0.0429	0.0424
2.00	0.0107	0.0294	0.0231	0.0242	0.0239

2.20	0.0053	0.0172	0.0129	0.0136	0.0134
2.40	0.0026	0.0100	0.0071	0.0076	0.0074
2.60	0.0013	0.0058	0.0039	0.0042	0.0041
2.80	0.0006	0.0033	0.0021	0.0023	0.0023
3.00	0.0003	0.0019	0.0012	0.0013	0.0013
3.20	0.	0.	0.	0.	0.
3.40	0.	0.	0.	0.	0.
3.60	0.	0.	0.	0.	0.
3.80	0.	0.	0.	0.	0.
4.00	0.	0.	0.	0.	0.
4.50	0.	0.	0.	0.	0.
5.00	0.	0.	0.	0.	0.
5.50	0.	0.	0.	0.	0.
6.00	0.	0.	0.	0.	0.
7.00	0.	0.	0.	0.	0.
8.00	0.	0.	0.	0.	0.
9.00	0.	0.	0.	0.	0.
10.00	0.	0.	0.	0.	0.
12.00	0.	0.	0.	0.	0.
14.00	0.	0.	0.	0.	0.
16.00	0.	0.	0.	0.	0.
18.00	0.	0.	0.	0.	0.

FOR NL-GROUP 1 , THE P(NL,R) ARE AS FOLLOWS

ITERATION= 6

R	
0.	0.
0.02	0.2766
0.04	0.5109
0.06	0.7077
0.08	0.8716
0.10	1.0065
0.12	1.1159
0.14	1.2031
0.16	1.2707
0.18	1.3213
0.20	1.3570
0.25	1.3989
0.30	1.3893
0.35	1.3442
0.40	1.2761
0.45	1.1942
0.50	1.1049
0.55	1.0129
0.60	0.9213
0.70	0.7500
0.80	0.6002
0.90	0.4742
1.00	0.3709
1.10	0.2878
1.20	0.2219
1.30	0.1703
1.40	0.1303
1.60	0.0749
1.80	0.0426
2.00	0.0240

2.20	0.0134
2.40	0.0075
2.60	0.0042
2.80	0.0023
3.00	0.0013
3.20	0.
3.40	0.
3.60	0.
3.80	0.
4.00	0.
4.50	0.
5.00	0.
5.50	0.
6.00	0.
7.00	0.
8.00	0.
9.00	0.
10.00	0.
12.00	0.
14.00	0.
16.00	0.
18.00	0.

FOR NL-GROUP 1 , THE ZO(NL,NL,R) ARE AS FOLLOWS

ITERATION=	1	2	3	4	5
R					
0.	0.	0.	0.	0.	0.
0.02	0.0009	0.0007	0.0008	0.0008	0.0008
0.04	0.0047	0.0040	0.0042	0.0041	0.0041
0.06	0.0134	0.0113	0.0118	0.0117	0.0118
0.08	0.0277	0.0235	0.0245	0.0243	0.0244
0.10	0.0478	0.0406	0.0424	0.0420	0.0421
0.12	0.0734	0.0625	0.0652	0.0645	0.0647
0.14	0.1038	0.0885	0.0923	0.0914	0.0917
0.16	0.1384	0.1181	0.1231	0.1220	0.1223
0.18	0.1762	0.1507	0.1570	0.1555	0.1559
0.20	0.2164	0.1855	0.1931	0.1914	0.1918
0.25	0.3221	0.2779	0.2886	0.2862	0.2869
0.30	0.4283	0.3729	0.3863	0.3833	0.3841
0.35	0.5281	0.4648	0.4801	0.4766	0.4775
0.40	0.6173	0.5498	0.5661	0.5624	0.5634
0.45	0.6944	0.6258	0.6426	0.6388	0.6398
0.50	0.7590	0.6922	0.7087	0.7050	0.7060
0.55	0.8120	0.7490	0.7647	0.7612	0.7621
0.60	0.8546	0.7968	0.8113	0.8081	0.8090
0.70	0.9156	0.8694	0.8814	0.8788	0.8795
0.80	0.9524	0.9177	0.9270	0.9250	0.9256
0.90	0.9737	0.9489	0.9559	0.9544	0.9548
1.00	0.9857	0.9686	0.9736	0.9726	0.9729
1.10	0.9923	0.9809	0.9844	0.9837	0.9839
1.20	0.9959	0.9884	0.9908	0.9903	0.9905
1.30	0.9978	0.9929	0.9946	0.9943	0.9944
1.40	0.9988	0.9957	0.9968	0.9966	0.9967
1.60	0.9997	0.9985	0.9990	0.9989	0.9989
1.80	0.9999	0.9995	0.9997	0.9996	0.9996
2.00	1.0000	0.9998	0.9999	0.9999	0.9999

2.20	1.0000	0.9999	1.0000	1.0000	1.0000
2.40	1.0000	1.0000	1.0000	1.0000	1.0000
2.60	1.0000	1.0000	1.0000	1.0000	1.0000
2.80	1.0000	1.0000	1.0000	1.0000	1.0000
3.00	1.0000	1.0000	1.0000	1.0000	1.0000
3.20	1.0000	1.0000	1.0000	1.0000	1.0000
3.40	1.0000	1.0000	1.0000	1.0000	1.0000
3.60	1.0000	1.0000	1.0000	1.0000	1.0000
3.80	1.0000	1.0000	1.0000	1.0000	1.0000
4.00	1.0000	1.0000	1.0000	1.0000	1.0000
4.50	1.0000	1.0000	1.0000	1.0000	1.0000
5.00	1.0000	1.0000	1.0000	1.0000	1.0000
5.50	1.0000	1.0000	1.0000	1.0000	1.0000
6.00	1.0000	1.0000	1.0000	1.0000	1.0000
7.00	1.0000	1.0000	1.0000	1.0000	1.0000
8.00	1.0000	1.0000	1.0000	1.0000	1.0000
9.00	1.0000	1.0000	1.0000	1.0000	1.0000
10.00	1.0000	1.0000	1.0000	1.0000	1.0000
12.00	1.0000	1.0000	1.0000	1.0000	1.0000
14.00	1.0000	1.0000	1.0000	1.0000	1.0000
16.00	1.0000	1.0000	1.0000	1.0000	1.0000
18.00	1.0000	1.0000	1.0000	1.0000	1.0000

FOR NL-GROUP 1 , THE ZO(NL,NL,R) ARE AS FOLLOWS

ITERATION= 6

R	
0.	0.
0.02	0.0008
0.04	0.0041
0.06	0.0118
0.08	0.0244
0.10	0.0421
0.12	0.0647
0.14	0.0916
0.16	0.1222
0.18	0.1558
0.20	0.1917
0.25	0.2867
0.30	0.3838
0.35	0.4773
0.40	0.5631
0.45	0.6395
0.50	0.7057
0.55	0.7619
0.60	0.8087
0.70	0.8793
0.80	0.9254
0.90	0.9547
1.00	0.9728
1.10	0.9838
1.20	0.9904
1.30	0.9943
1.40	0.9966
1.60	0.9989
1.80	0.9996
2.00	0.9999

2.20	1.0000
2.40	1.0000
2.60	1.0000
2.80	1.0000
3.00	1.0000
3.20	1.0000
3.40	1.0000
3.60	1.0000
3.80	1.0000
4.00	1.0000
4.50	1.0000
5.00	1.0000
5.50	1.0000
6.00	1.0000
7.00	1.0000
8.00	1.0000
9.00	1.0000
10.00	1.0000
12.00	1.0000
14.00	1.0000
16.00	1.0000
18.00	1.0000

FOR NL-GROUP 1 , THE YO(NL,NL,R) ARE AS FOLLOWS

ITERATION=	1	2	3	4	5
R					
0.	0.	0.	0.	0.	0.
0.02	0.0720	0.0661	0.0676	0.0672	0.0673
0.04	0.1431	0.1315	0.1344	0.1337	0.1339
0.06	0.2123	0.1953	0.1995	0.1985	0.1988
0.08	0.2786	0.2566	0.2620	0.2608	0.2612
0.10	0.3414	0.3149	0.3214	0.3199	0.3203
0.12	0.4001	0.3697	0.3772	0.3755	0.3760
0.14	0.4545	0.4209	0.4292	0.4274	0.4279
0.16	0.5046	0.4684	0.4774	0.4753	0.4759
0.18	0.5504	0.5122	0.5216	0.5195	0.5201
0.20	0.5920	0.5524	0.5622	0.5600	0.5606
0.25	0.6859	0.6441	0.6544	0.6521	0.6527
0.30	0.7587	0.7173	0.7276	0.7253	0.7259
0.35	0.8137	0.7747	0.7845	0.7823	0.7829
0.40	0.8545	0.8190	0.8280	0.8260	0.8265
0.45	0.8842	0.8526	0.8607	0.8589	0.8594
0.50	0.9053	0.8778	0.8849	0.8834	0.8838
0.55	0.9199	0.8964	0.9025	0.9012	0.9016
0.60	0.9297	0.9098	0.9151	0.9139	0.9142
0.70	0.9422	0.9286	0.9324	0.9316	0.9318
0.80	0.9460	0.9371	0.9396	0.9391	0.9393
0.90	0.9452	0.9395	0.9412	0.9409	0.9410
1.00	0.9421	0.9385	0.9396	0.9394	0.9394
1.10	0.9377	0.9355	0.9362	0.9361	0.9361
1.20	0.9327	0.9313	0.9318	0.9317	0.9317
1.30	0.9274	0.9266	0.9269	0.9268	0.9269
1.40	0.9220	0.9215	0.9217	0.9216	0.9217
1.60	0.9111	0.9109	0.9110	0.9109	0.9109
1.80	0.9000	0.8999	0.9000	0.8999	0.8999
2.00	0.8889	0.8889	0.8889	0.8889	0.8889

2.20	0.8778	0.8778	0.8778	0.8778	0.8778
2.40	0.8667	0.8667	0.8667	0.8667	0.8667
2.60	0.8556	0.8555	0.8556	0.8556	0.8556
2.80	0.8444	0.8444	0.8444	0.8444	0.8444
3.00	0.8333	0.8333	0.8333	0.8333	0.8333
3.20	0.8222	0.8222	0.8222	0.8222	0.8222
3.40	0.8111	0.8111	0.8111	0.8111	0.8111
3.60	0.8000	0.8000	0.8000	0.8000	0.8000
3.80	0.7889	0.7889	0.7889	0.7889	0.7889
4.00	0.7778	0.7778	0.7778	0.7778	0.7778
4.50	0.7500	0.7500	0.7500	0.7500	0.7500
5.00	0.7222	0.7222	0.7222	0.7222	0.7222
5.50	0.6944	0.6944	0.6944	0.6944	0.6944
6.00	0.6667	0.6667	0.6667	0.6667	0.6667
7.00	0.6111	0.6111	0.6111	0.6111	0.6111
8.00	0.5556	0.5556	0.5556	0.5556	0.5556
9.00	0.5000	0.5000	0.5000	0.5000	0.5000
10.00	0.4444	0.4444	0.4444	0.4444	0.4444
12.00	0.3333	0.3333	0.3333	0.3333	0.3333
14.00	0.2222	0.2222	0.2222	0.2222	0.2222
16.00	0.1111	0.1111	0.1111	0.1111	0.1111
18.00	0.	0.	0.	0.	0.

FOR NL-GROUP 1 , THE Y(NL,R) ARE AS FOLLOWS

ITERATION= R	1	2	3	4	5
0.	4.0000	4.0000	4.0000	4.0000	4.0000
0.02	3.9084	3.9327	3.9267	3.9284	3.9279
0.04	3.8169	3.8655	3.8534	3.8568	3.8558
0.06	3.7265	3.7990	3.7809	3.7860	3.7845
0.08	3.6383	3.7339	3.7100	3.7167	3.7148
0.10	3.5532	3.6709	3.6414	3.6497	3.6473
0.12	3.4719	3.6106	3.5757	3.5855	3.5827
0.14	3.3948	3.5532	3.5132	3.5245	3.5212
0.16	3.3222	3.4989	3.4542	3.4669	3.4632
0.18	3.2542	3.4480	3.3987	3.4127	3.4086
0.20	3.0330	3.2685	3.2082	3.2253	3.2203
0.25	2.8827	3.1554	3.0850	3.1050	3.0992
0.30	2.7513	3.0563	2.9771	2.9996	2.9930
0.35	2.6361	2.9701	2.8828	2.9077	2.9004
0.40	2.5341	2.8950	2.8003	2.8273	2.8194
0.45	2.4424	2.8291	2.7275	2.7565	2.7480
0.50	2.3584	2.7707	2.6624	2.6934	2.6843
0.55	2.2803	2.7184	2.6033	2.6363	2.6266
0.60	2.1230	2.6097	2.4820	2.5187	2.5079
0.70	1.9814	2.5206	2.3793	2.4200	2.4081
0.80	1.8496	2.4400	2.2848	2.3295	2.3164
0.90	1.7269	2.3644	2.1954	2.2441	2.2298
1.00	1.6141	2.2921	2.1094	2.1620	2.1465
1.10	1.5123	2.2219	2.0262	2.0825	2.0660
1.20	1.4219	2.1535	1.9459	2.0055	1.9880
1.30	1.3433	2.0868	1.8686	1.9311	1.9127
1.40	1.2142	1.9617	1.7259	1.7930	1.7732
1.60	1.0995	1.8349	1.5847	1.6555	1.6346
1.80	1.0175	1.7156	1.4581	1.5303	1.5089
2.00	0.9601	1.6049	1.3467	1.4184	1.3971

2.20	0.9200	1.5033	1.2505	1.3199	1.2991
2.40	0.8912	1.4112	1.1684	1.2342	1.2144
2.60	0.8696	1.3283	1.0990	1.1603	1.1417
2.80	0.8524	1.2544	1.0407	1.0970	1.0798
3.00	0.8379	1.1887	0.9918	1.0428	1.0271
3.20	0.8248	1.1307	0.9508	0.9967	0.9825
3.40	0.8127	1.0796	0.9162	0.9572	0.9444
3.60	0.8010	1.0347	0.8868	0.9234	0.9119
3.80	0.7896	0.9953	0.8617	0.8942	0.8840
4.00	0.7781	0.9251	0.8238	0.8475	0.8399
4.50	0.7501	0.8479	0.7753	0.7914	0.7862
5.00	0.7222	0.7885	0.7368	0.7477	0.7441
5.50	0.6944	0.7412	0.7036	0.7112	0.7086
6.00	0.6667	0.6899	0.6704	0.6740	0.6728
7.00	0.6111	0.6199	0.6121	0.6133	0.6129
8.00	0.5556	0.5591	0.5558	0.5563	0.5561
9.00	0.5000	0.5017	0.5001	0.5003	0.5002
10.00	0.4444	0.4450	0.4445	0.4445	0.4445
12.00	0.3333	0.3334	0.3333	0.3333	0.3333
14.00	0.2222	0.2222	0.2222	0.2222	0.2222
16.00	0.1111	0.1111	0.1111	0.1111	0.1111
18.00	0.	0.	0.	0.	0.

FOR NL-GROUP 2 , THE P(NL,R) ARE AS FOLLOWS

ITERATION=	1	2	3	4	5
R					
0.	0.	0.	0.	0.	0.
0.02	0.1043	0.0431	0.0595	0.0550	0.0563
0.04	0.1921	0.0796	0.1099	0.1014	0.1040
0.06	0.2649	0.1101	0.1520	0.1403	0.1438
0.08	0.3239	0.1355	0.1868	0.1725	0.1768
0.10	0.3704	0.1562	0.2151	0.1987	0.2036
0.12	0.4058	0.1728	0.2376	0.2196	0.2250
0.14	0.4309	0.1858	0.2550	0.2358	0.2415
0.16	0.4468	0.1956	0.2678	0.2477	0.2537
0.18	0.4546	0.2025	0.2765	0.2559	0.2621
0.20	0.4549	0.2068	0.2817	0.2609	0.2671
0.25	0.4288	0.2094	0.2822	0.2620	0.2681
0.30	0.3725	0.2021	0.2686	0.2501	0.2558
0.35	0.2949	0.1875	0.2444	0.2286	0.2335
0.40	0.2033	0.1675	0.2125	0.2001	0.2040
0.45	0.1035	0.1435	0.1751	0.1664	0.1692
0.50	0.	0.1167	0.1339	0.1291	0.1308
0.55	-0.1035	0.0878	0.0900	0.0894	0.0899
0.60	-0.2044	0.0577	0.0447	0.0482	0.0475
0.70	-0.3905	-0.0042	-0.0470	-0.0353	-0.0384
0.80	-0.5481	-0.0659	-0.1365	-0.1172	-0.1226
0.90	-0.6731	-0.1255	-0.2209	-0.1948	-0.2023
1.00	-0.7654	-0.1818	-0.2983	-0.2665	-0.2756
1.10	-0.8272	-0.2339	-0.3676	-0.3311	-0.3417
1.20	-0.8620	-0.2816	-0.4282	-0.3882	-0.3999
1.30	-0.8738	-0.3245	-0.4802	-0.4377	-0.4501
1.40	-0.8667	-0.3629	-0.5235	-0.4797	-0.4925
1.60	-0.8115	-0.4271	-0.5879	-0.5442	-0.5570
1.80	-0.7232	-0.4758	-0.6254	-0.5851	-0.5970
2.00	-0.6215	-0.5108	-0.6409	-0.6065	-0.6167

2.20	-0.5194	-0.5338	-0.6390	-0.6120	-0.6203
2.40	-0.4245	-0.5467	-0.6239	-0.6055	-0.6114
2.60	-0.3407	-0.5511	-0.5994	-0.5897	-0.5932
2.80	-0.2694	-0.5483	-0.5683	-0.5673	-0.5684
3.00	-0.2103	-0.5397	-0.5332	-0.5403	-0.5390
3.20	-0.1624	-0.5265	-0.4957	-0.5102	-0.5067
3.40	-0.1242	-0.5096	-0.4574	-0.4783	-0.4730
3.60	-0.0942	-0.4899	-0.4193	-0.4457	-0.4388
3.80	-0.0710	-0.4682	-0.3822	-0.4131	-0.4048
4.00	-0.0531	-0.4451	-0.3466	-0.3810	-0.3716
4.50	-0.0251	-0.3855	-0.2671	-0.3066	-0.2955
5.00	-0.0116	-0.3266	-0.2024	-0.2424	-0.2309
5.50	-0.0052	-0.2720	-0.1514	-0.1890	-0.1780
6.00	-0.0023	-0.2234	-0.1123	-0.1459	-0.1359
7.00	-0.0004	-0.1455	-0.0597	-0.0841	-0.0767
8.00	-0.0001	-0.0920	-0.0311	-0.0473	-0.0422
9.00	-0.0000	-0.0570	-0.0160	-0.0262	-0.0229
10.00	-0.	-0.0351	-0.0083	-0.0146	-0.0125
12.00	-0.	-0.0125	-0.0022	-0.0043	-0.0036
14.00	-0.	-0.0043	-0.0005	-0.0012	-0.0010
16.00	-0.	-0.0014	-0.0001	-0.0003	-0.0003
18.00	0.	0.	0.	0.	0.

FOR NL-GROUP 2 , THE P(NL,R) ARE AS FOLLOWS

ITERATION= 6

R	
0.	0.
0.02	0.0560
0.04	0.1033
0.06	0.1429
0.08	0.1757
0.10	0.2023
0.12	0.2236
0.14	0.2400
0.16	0.2521
0.18	0.2605
0.20	0.2655
0.25	0.2665
0.30	0.2543
0.35	0.2322
0.40	0.2030
0.45	0.1685
0.50	0.1304
0.55	0.0898
0.60	0.0478
0.70	-0.0375
0.80	-0.1211
0.90	-0.2002
1.00	-0.2731
1.10	-0.3388
1.20	-0.3967
1.30	-0.4468
1.40	-0.4891
1.60	-0.5537
1.80	-0.5940
2.00	-0.6142

2.20	-0.6183
2.40	-0.6099
2.60	-0.5923
2.80	-0.5681
3.00	-0.5393
3.20	-0.5076
3.40	-0.4744
3.60	-0.4406
3.80	-0.4069
4.00	-0.3740
4.50	-0.2984
5.00	-0.2339
5.50	-0.1809
6.00	-0.1386
7.00	-0.0786
8.00	-0.0435
9.00	-0.0238
10.00	-0.0131
12.00	-0.0038
14.00	-0.0011
16.00	-0.0003
18.00	0.

FOR NL-GROUP 2 , THE ZO(NL,NL,R) ARE AS FOLLOWS

ITERATION=	1	2	3	4	5
R					
0.	0.	0.	0.	0.	0.
0.02	0.0001	0.0000	0.0000	0.0000	0.0000
0.04	0.0006	0.0001	0.0002	0.0002	0.0002
0.06	0.0017	0.0003	0.0005	0.0005	0.0005
0.08	0.0034	0.0006	0.0011	0.0010	0.0010
0.10	0.0058	0.0010	0.0019	0.0016	0.0017
0.12	0.0088	0.0016	0.0030	0.0025	0.0026
0.14	0.0123	0.0022	0.0042	0.0036	0.0037
0.16	0.0162	0.0029	0.0055	0.0047	0.0050
0.18	0.0203	0.0037	0.0070	0.0060	0.0063
0.20	0.0244	0.0046	0.0086	0.0073	0.0077
0.25	0.0342	0.0067	0.0126	0.0108	0.0113
0.30	0.0422	0.0088	0.0164	0.0140	0.0147
0.35	0.0479	0.0107	0.0196	0.0169	0.0177
0.40	0.0511	0.0123	0.0223	0.0192	0.0201
0.45	0.0524	0.0135	0.0242	0.0209	0.0219
0.50	0.0527	0.0144	0.0254	0.0220	0.0230
0.55	0.0529	0.0149	0.0260	0.0226	0.0236
0.60	0.0542	0.0152	0.0263	0.0229	0.0239
0.70	0.0640	0.0154	0.0265	0.0231	0.0241
0.80	0.0866	0.0156	0.0275	0.0238	0.0249
0.90	0.1243	0.0166	0.0309	0.0264	0.0277
1.00	0.1762	0.0190	0.0378	0.0318	0.0336
1.10	0.2397	0.0234	0.0490	0.0409	0.0432
1.20	0.3111	0.0301	0.0649	0.0539	0.0570
1.30	0.3864	0.0393	0.0856	0.0710	0.0751
1.40	0.4622	0.0512	0.1109	0.0921	0.0974
1.60	0.6031	0.0826	0.1728	0.1447	0.1527
1.80	0.7213	0.1235	0.2465	0.2086	0.2194
2.00	0.8123	0.1722	0.3267	0.2796	0.2930

2.20	0.8779	0.2268	0.4086	0.3538	0.3695
2.40	0.9229	0.2852	0.4884	0.4279	0.4454
2.60	0.9525	0.3455	0.5632	0.4994	0.5179
2.80	0.9714	0.4059	0.6314	0.5663	0.5854
3.00	0.9830	0.4651	0.6922	0.6277	0.6468
3.20	0.9901	0.5220	0.7452	0.6829	0.7015
3.40	0.9943	0.5757	0.7907	0.7318	0.7496
3.60	0.9967	0.6256	0.8292	0.7746	0.7912
3.80	0.9981	0.6716	0.8614	0.8115	0.8268
4.00	0.9989	0.7133	0.8880	0.8431	0.8570
4.50	0.9998	0.8000	0.9359	0.9029	0.9134
5.00	0.9999	0.8638	0.9639	0.9411	0.9485
5.50	1.0000	0.9090	0.9799	0.9647	0.9698
6.00	1.0000	0.9400	0.9888	0.9790	0.9823
7.00	1.0000	0.9755	0.9969	0.9932	0.9945
8.00	1.0000	0.9903	0.9991	0.9978	0.9983
9.00	1.0000	0.9962	0.9998	0.9993	0.9995
10.00	1.0000	0.9984	0.9999	0.9997	0.9998
12.00	1.0000	0.9998	1.0000	1.0000	1.0000
14.00	1.0000	1.0000	1.0000	1.0000	1.0000
16.00	1.0000	1.0000	1.0000	1.0000	1.0000
18.00	1.0000	1.0000	1.0000	1.0000	1.0000

FOR NL-GROUP 2 , THE ZO(NL,NL,R) ARE AS FOLLOWS

ITERATION= 6

R	
0.	0.
0.02	0.0000
0.04	0.0002
0.06	0.0005
0.08	0.0010
0.10	0.0017
0.12	0.0026
0.14	0.0037
0.16	0.0049
0.18	0.0062
0.20	0.0076
0.25	0.0111
0.30	0.0145
0.35	0.0175
0.40	0.0199
0.45	0.0216
0.50	0.0227
0.55	0.0234
0.60	0.0236
0.70	0.0238
0.80	0.0246
0.90	0.0274
1.00	0.0331
1.10	0.0426
1.20	0.0562
1.30	0.0740
1.40	0.0960
1.60	0.1505
1.80	0.2165
2.00	0.2895

2.20	0.3654
2.40	0.4409
2.60	0.5132
2.80	0.5805
3.00	0.6419
3.20	0.6967
3.40	0.7450
3.60	0.7869
3.80	0.8229
4.00	0.8534
4.50	0.9107
5.00	0.9466
5.50	0.9685
6.00	0.9815
7.00	0.9942
8.00	0.9982
9.00	0.9994
10.00	0.9998
12.00	1.0000
14.00	1.0000
16.00	1.0000
18.00	1.0000

FOR NL-GROUP 2 , THE YO(NL,NL,R) ARE AS FOLLOWS

ITERATION=	1	2	3	4	5
R					
0.	0.	0.	0.	0.	0.
0.02	0.0176	0.0069	0.0095	0.0088	0.0090
0.04	0.0351	0.0138	0.0190	0.0175	0.0179
0.06	0.0523	0.0206	0.0285	0.0261	0.0268
0.08	0.0692	0.0274	0.0378	0.0347	0.0356
0.10	0.0856	0.0341	0.0470	0.0431	0.0443
0.12	0.1016	0.0407	0.0560	0.0514	0.0528
0.14	0.1171	0.0472	0.0648	0.0596	0.0611
0.16	0.1320	0.0536	0.0735	0.0676	0.0693
0.18	0.1465	0.0600	0.0819	0.0755	0.0774
0.20	0.1605	0.0662	0.0903	0.0832	0.0853
0.25	0.1946	0.0816	0.1107	0.1021	0.1047
0.30	0.2266	0.0966	0.1303	0.1204	0.1233
0.35	0.2574	0.1112	0.1493	0.1382	0.1414
0.40	0.2873	0.1256	0.1678	0.1555	0.1591
0.45	0.3168	0.1397	0.1860	0.1725	0.1765
0.50	0.3462	0.1538	0.2040	0.1894	0.1937
0.55	0.3756	0.1677	0.2219	0.2061	0.2107
0.60	0.4049	0.1816	0.2397	0.2228	0.2277
0.70	0.4633	0.2093	0.2752	0.2561	0.2617
0.80	0.5204	0.2370	0.3108	0.2894	0.2956
0.90	0.5746	0.2647	0.3462	0.3226	0.3295
1.00	0.6247	0.2923	0.3812	0.3555	0.3630
1.10	0.6695	0.3196	0.4155	0.3879	0.3960
1.20	0.7086	0.3465	0.4489	0.4194	0.4280
1.30	0.7417	0.3729	0.4809	0.4499	0.4590
1.40	0.7690	0.3985	0.5113	0.4790	0.4885
1.60	0.8129	0.4482	0.5685	0.5343	0.5443
1.80	0.8391	0.4938	0.6179	0.5830	0.5933
2.00	0.8522	0.5350	0.6592	0.6246	0.6348

2.20	0.8562	0.5713	0.6924	0.6591	0.6690
2.40	0.8542	0.6026	0.7182	0.6868	0.6963
2.60	0.8485	0.6290	0.7374	0.7084	0.7172
2.80	0.8405	0.6509	0.7508	0.7245	0.7325
3.00	0.8311	0.6683	0.7593	0.7357	0.7430
3.20	0.8210	0.6819	0.7638	0.7430	0.7494
3.40	0.8104	0.6919	0.7649	0.7467	0.7524
3.60	0.7996	0.6987	0.7634	0.7476	0.7526
3.80	0.7886	0.7028	0.7598	0.7461	0.7504
4.00	0.7776	0.7044	0.7544	0.7426	0.7464
4.50	0.7500	0.7033	0.7377	0.7301	0.7326
5.00	0.7222	0.6926	0.7157	0.7109	0.7125
5.50	0.6944	0.6755	0.6909	0.6878	0.6889
6.00	0.6667	0.6542	0.6646	0.6627	0.6633
7.00	0.6111	0.6066	0.6106	0.6100	0.6102
8.00	0.5556	0.5539	0.5554	0.5552	0.5553
9.00	0.5000	0.4994	0.5000	0.4999	0.4999
10.00	0.4444	0.4441	0.4444	0.4444	0.4444
12.00	0.3333	0.3333	0.3333	0.3333	0.3333
14.00	0.2222	0.2222	0.2222	0.2222	0.2222
16.00	0.1111	0.1111	0.1111	0.1111	0.1111
18.00	0.	0.	0.	0.	0.

FOR NL-GROUP 2 , THE Y(NL,R) ARE AS FOLLOWS

ITERATION=	1	2	3	4	5
R					
0.	4.0000	4.0000	4.0000	4.0000	4.0000
0.02	3.8540	3.8735	3.8686	3.8699	3.8695
0.04	3.7089	3.7478	3.7381	3.7406	3.7399
0.06	3.5665	3.6243	3.6099	3.6136	3.6126
0.08	3.4288	3.5047	3.4857	3.4906	3.4892
0.10	3.2975	3.3901	3.3669	3.3730	3.3712
0.12	3.1734	3.2815	3.2544	3.2615	3.2595
0.14	3.0573	3.1794	3.1488	3.1568	3.1545
0.16	2.9496	3.0841	3.0503	3.0591	3.0566
0.18	2.8503	2.9957	2.9590	2.9686	2.9659
0.20	2.6016	2.7824	2.7363	2.7485	2.7450
0.25	2.3914	2.5929	2.5413	2.5550	2.5511
0.30	2.2192	2.4356	2.3798	2.3947	2.3904
0.35	2.0798	2.3066	2.2477	2.2635	2.2590
0.40	1.9669	2.2016	2.1402	2.1568	2.1520
0.45	1.8751	2.1162	2.0528	2.0701	2.0651
0.50	1.7994	2.0467	1.9814	1.9994	1.9941
0.55	1.7359	1.9897	1.9226	1.9412	1.9357
0.60	1.5981	1.8815	1.8066	1.8275	1.8214
0.70	1.5026	1.8013	1.7222	1.7445	1.7380
0.80	1.4240	1.7399	1.6559	1.6798	1.6728
0.90	1.3563	1.6896	1.6003	1.6258	1.6183
1.00	1.2967	1.6459	1.5510	1.5781	1.5701
1.10	1.2441	1.6061	1.5056	1.5343	1.5259
1.20	1.1978	1.5687	1.4630	1.4932	1.4843
1.30	1.1576	1.5331	1.4226	1.4541	1.4448
1.40	1.0612	1.4388	1.3155	1.3504	1.3400
1.60	1.0013	1.3722	1.2422	1.2788	1.2680
1.80	0.9566	1.3095	1.1760	1.2133	1.2022
2.00	0.9234	1.2510	1.1170	1.1541	1.1430

2.20	0.8983	1.1968	1.0652	1.1012	1.0904
2.40	0.8787	1.1471	1.0200	1.0543	1.0440
2.60	0.8625	1.1018	0.9809	1.0131	1.0033
2.80	0.8485	1.0608	0.9470	0.9770	0.9678
3.00	0.8357	1.0237	0.9178	0.9453	0.9368
3.20	0.8236	0.9904	0.8923	0.9174	0.9096
3.40	0.8120	0.9604	0.8700	0.8928	0.8857
3.60	0.8006	0.9335	0.8503	0.8710	0.8645
3.80	0.7893	0.9092	0.8326	0.8514	0.8455
4.00	0.7779	0.8518	0.8004	0.8124	0.8086
4.50	0.7500	0.8012	0.7631	0.7715	0.7688
5.00	0.7222	0.7589	0.7303	0.7364	0.7344
5.50	0.6944	0.7222	0.7000	0.7046	0.7031
6.00	0.6667	0.6774	0.6684	0.6700	0.6695
7.00	0.6111	0.6154	0.6116	0.6122	0.6120
8.00	0.5556	0.5575	0.5557	0.5559	0.5558
9.00	0.5000	0.5011	0.5001	0.5002	0.5001
10.00	0.4444	0.4447	0.4445	0.4445	0.4445
12.00	0.3333	0.3334	0.3333	0.3333	0.3333
14.00	0.2222	0.2222	0.2222	0.2222	0.2222
16.00	0.1111	0.1111	0.1111	0.1111	0.1111
18.00	0.	0.	0.	0.	0.

THE Y(R) ARE AS FOLLOWS

ITERATION=	1	2	3	4	5
R					
0.02	4.0000	4.0000	4.0000	4.0000	4.0000
0.04	3.8364	3.8666	3.8591	3.8611	3.8605
0.06	3.6738	3.7340	3.7190	3.7231	3.7219
0.08	3.5142	3.6037	3.5814	3.5875	3.5857
0.10	3.3596	3.4773	3.4479	3.4559	3.4536
0.12	3.2118	3.3560	3.3200	3.3298	3.3270
0.14	3.0718	3.2408	3.1985	3.2100	3.2067
0.16	2.9403	3.1322	3.0840	3.0972	3.0934
0.18	2.8176	3.0305	2.9768	2.9915	2.9873
0.20	2.7038	2.9358	2.8771	2.8932	2.8885
0.25	2.4410	2.7162	2.6460	2.6653	2.6598
0.30	2.1968	2.5113	2.4306	2.4529	2.4464
0.35	1.9926	2.3390	2.2495	2.2743	2.2671
0.40	1.8224	2.1954	2.0984	2.1254	2.1175
0.45	1.6796	2.0760	1.9724	2.0014	1.9929
0.50	1.5582	1.9764	1.8668	1.8976	1.8886
0.55	1.4532	1.8929	1.7774	1.8100	1.8005
0.60	1.3604	1.8220	1.7007	1.7350	1.7250
0.70	1.1932	1.6999	1.5669	1.6048	1.5937
0.80	1.0392	1.5920	1.4469	1.4884	1.4763
0.90	0.9036	1.5029	1.3452	1.3904	1.3771
1.00	0.7817	1.4249	1.2541	1.3032	1.2888
1.10	0.6721	1.3536	1.1698	1.2226	1.2071
1.20	0.5746	1.2865	1.0900	1.1464	1.1299
1.30	0.4892	1.2222	1.0141	1.0738	1.0562
1.40	0.4159	1.1602	0.9417	1.0042	0.9858
1.60	0.2922	1.0402	0.8042	0.8714	0.8516
1.80	0.1884	0.9240	0.6738	0.7445	0.7236
2.00	0.1175	0.8157	0.5581	0.6304	0.6089
2.20	0.0712	0.7160	0.4579	0.5295	0.5082

2.40	0.0422	0.6255	0.3727	0.4421	0.4213
2.60	0.0245	0.5445	0.3017	0.3675	0.3477
2.80	0.0140	0.4728	0.2435	0.3047	0.2861
3.00	0.0080	0.4099	0.1963	0.2525	0.2353
3.20	0.0045	0.3554	0.1585	0.2095	0.1938
3.40	0.0026	0.3085	0.1285	0.1745	0.1602
3.60	0.0016	0.2685	0.1051	0.1461	0.1333
3.80	0.0010	0.2347	0.0868	0.1234	0.1119
4.00	0.0007	0.2064	0.0728	0.1054	0.0951
4.50	0.0003	0.1473	0.0460	0.0698	0.0622
5.00	0.0001	0.0979	0.0253	0.0414	0.0362
5.50	0.0000	0.0663	0.0146	0.0255	0.0219
6.00	0.	0.0468	0.0091	0.0167	0.0142
7.00	0.	0.0232	0.0037	0.0074	0.0061
8.00	0.	0.0088	0.0010	0.0022	0.0018
9.00	0.	0.0036	0.0003	0.0007	0.0006
10.00	0.	0.0017	0.0001	0.0003	0.0002
12.00	0.	0.0005	0.0000	0.0001	0.0001
14.00	0.	0.0001	0.	0.0000	0.
16.00	0.	0.0000	0.	0.	0.
18.00	0.	0.	0.	0.	0.

THE Z(R) ARE AS FOLLOWS

ITERATION=	1	2	3	4	5
R					
0.	4.0000	4.0000	4.0000	4.0000	4.0000
0.02	3.9980	3.9985	3.9984	3.9984	3.9984
0.04	3.9894	3.9918	3.9913	3.9914	3.9914
0.06	3.9699	3.9767	3.9752	3.9756	3.9755
0.08	3.9378	3.9518	3.9486	3.9494	3.9492
0.10	3.8927	3.9167	3.9113	3.9127	3.9123
0.12	3.8355	3.8720	3.8637	3.8658	3.8652
0.14	3.7677	3.8186	3.8071	3.8100	3.8092
0.16	3.6909	3.7578	3.7426	3.7465	3.7454
0.18	3.6071	3.6911	3.6720	3.6769	3.6755
0.20	3.5183	3.6198	3.5966	3.6026	3.6009
0.25	3.2875	3.4307	3.3976	3.4061	3.4037
0.30	3.0589	3.2365	3.1947	3.2054	3.2024
0.35	2.8481	3.0489	3.0005	3.0130	3.0095
0.40	2.6631	2.8758	2.8231	2.8367	2.8329
0.45	2.5065	2.7212	2.6665	2.6806	2.6766
0.50	2.3767	2.5867	2.5319	2.5460	2.5420
0.55	2.2702	2.4721	2.4186	2.4324	2.4284
0.60	2.1822	2.3761	2.3248	2.3380	2.3342
0.70	2.0408	2.2304	2.1842	2.1963	2.1928
0.80	1.9220	2.1333	2.0908	2.1023	2.0990
0.90	1.8040	2.0689	2.0265	2.0384	2.0349
1.00	1.6761	2.0247	1.9771	1.9911	1.9871
1.10	1.5358	1.9914	1.9332	1.9508	1.9458
1.20	1.3859	1.9630	1.8885	1.9115	1.9050
1.30	1.2315	1.9354	1.8395	1.8694	1.8610
1.40	1.0780	1.9062	1.7846	1.8226	1.8118
1.60	0.7943	1.8378	1.6564	1.7128	1.6968
1.80	0.5575	1.7540	1.5076	1.5836	1.5620
2.00	0.3755	1.6559	1.3468	1.4411	1.4142

2.20	0.2443	1.5465	1.1828	1.2924	1.2610
2.40	0.1543	1.4296	1.0233	1.1441	1.1093
2.60	0.0950	1.3090	0.8736	1.0012	0.9641
2.80	0.0573	1.1882	0.7371	0.8673	0.8291
3.00	0.0339	1.0698	0.6157	0.7446	0.7064
3.20	0.0198	0.9560	0.5097	0.6341	0.5969
3.40	0.0114	0.8487	0.4187	0.5363	0.5008
3.60	0.0066	0.7487	0.3416	0.4508	0.4176
3.80	0.0038	0.6569	0.2773	0.3769	0.3463
4.00	0.0022	0.5734	0.2240	0.3138	0.2859
4.50	0.0005	0.4000	0.1283	0.1942	0.1733
5.00	0.0001	0.2723	0.0721	0.1178	0.1030
5.50	0.0000	0.1820	0.0402	0.0705	0.0605
6.00	0.0000	0.1201	0.0224	0.0420	0.0354
7.00	0.	0.0490	0.0062	0.0136	0.0110
8.00	0.	0.0193	0.0017	0.0043	0.0034
9.00	0.	0.0076	0.0005	0.0014	0.0010
10.00	0.	0.0032	0.0002	0.0005	0.0004
12.00	0.	0.0004	0.0000	0.0000	0.0000
14.00	0.	0.0000	0.	0.	0.
16.00	0.	0.	0.	0.	0.
18.00	0.	0.	0.	0.	0.

THE Z(R) ARE AS FOLLOWS

ITERATION= 6

R	
0.	4.0000
0.02	3.9984
0.04	3.9914
0.06	3.9755
0.08	3.9493
0.10	3.9124
0.12	3.8654
0.14	3.8094
0.16	3.7457
0.18	3.6759
0.20	3.6014
0.25	3.4044
0.30	3.2032
0.35	3.0105
0.40	2.8339
0.45	2.6777
0.50	2.5431
0.55	2.4295
0.60	2.3353
0.70	2.1938
0.80	2.0999
0.90	2.0359
1.00	1.9882
1.10	1.9472
1.20	1.9068
1.30	1.8632
1.40	1.8148
1.60	1.7011
1.80	1.5677
2.00	1.4212

2.20	1.2692
2.40	1.1183
2.60	0.9737
2.80	0.8390
3.00	0.7162
3.20	0.6065
3.40	0.5100
3.60	0.4261
3.80	0.3542
4.00	0.2931
4.50	0.1786
5.00	0.1067
5.50	0.0630
6.00	0.0371
7.00	0.0117
8.00	0.0036
9.00	0.0011
10.00	0.0004
12.00	0.0000
14.00	0.
16.00	0.
18.00	0.

CALCULATION OF ATOMIC STRUCTURE CONATSER

INPUT FOR NEXT CALCULATIONS WERE

ATOM = BERYLLIUM

NGR = 2

IDIM =150

ALPHA = 2.000000

ZTEST = 0.010000

TNORM = 0.000100

TD2P = 0.010000

XTEST = 0.001000

PTEST = 0.010000

IRMAX(1)= 36

IRO(1)= 12

Q(1)= 2.0000

AIN(1)= 0.000700

IRMAX(2)= 52

IRO(2)= 30

Q(2)= 2.0000

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AIN(  2)= -0.000100
E( 1 )=  0.800000E 01
E( 2 )=  0.200000E-00
```

ATOMIC STRUCTURE FOR BERYLLIUM

AFTER 6 ITERATIONS ON THE P-S AND 10 ITERATIONS ON THE E-S

THE CALCULATED E-S FOR THE NL-GROUPS ARE

E(1)= 0.974698E 01

E(2)= 0.490867E-00

FOR NL-GROUP 1 , THE P(NL,R) ARE AS FOLLOWS

ITERATION=	1	2	3	4	5
R					
0.	0.	0.	0.	0.	0.
0.02	0.2952	0.2717	0.2777	0.2763	0.2767
0.04	0.5449	0.5018	0.5129	0.5104	0.5111
0.06	0.7546	0.6952	0.7105	0.7070	0.7080
0.08	0.9287	0.8564	0.8750	0.8707	0.8719
0.10	1.0717	0.9892	1.0103	1.0055	1.0068
0.12	1.1871	1.0972	1.1201	1.1149	1.1163
0.14	1.2785	1.1835	1.2075	1.2020	1.2035
0.16	1.3488	1.2506	1.2752	1.2696	1.2712
0.18	1.4007	1.3011	1.3259	1.3202	1.3218
0.20	1.4367	1.3371	1.3616	1.3559	1.3575
0.25	1.4703	1.3813	1.4029	1.3980	1.3993
0.30	1.4446	1.3755	1.3924	1.3885	1.3896
0.35	1.3798	1.3350	1.3462	1.3437	1.3444
0.40	1.2911	1.2716	1.2770	1.2759	1.2762
0.45	1.1892	1.1942	1.1940	1.1942	1.1942
0.50	1.0818	1.1090	1.1038	1.1051	1.1048
0.55	0.9743	1.0205	1.0109	1.0133	1.0127
0.60	0.8702	0.9318	0.9187	0.9219	0.9211
0.70	0.6805	0.7648	0.7465	0.7509	0.7497
0.80	0.5213	0.6175	0.5962	0.6012	0.5998
0.90	0.3931	0.4925	0.4700	0.4752	0.4738
1.00	0.2928	0.3893	0.3668	0.3719	0.3704
1.10	0.2159	0.3055	0.2839	0.2887	0.2874
1.20	0.1579	0.2385	0.2184	0.2228	0.2216
1.30	0.1146	0.1855	0.1673	0.1711	0.1700
1.40	0.0828	0.1439	0.1277	0.1310	0.1301
1.60	0.0425	0.0854	0.0730	0.0754	0.0747
1.80	0.0215	0.0502	0.0413	0.0429	0.0424
2.00	0.0107	0.0294	0.0231	0.0242	0.0239

2.20	0.0053	0.0172	0.0128	0.0136	0.0134
2.40	0.0026	0.0100	0.0071	0.0076	0.0074
2.60	0.0013	0.0058	0.0039	0.0042	0.0041
2.80	0.0006	0.0033	0.0021	0.0023	0.0023
3.00	0.0003	0.0019	0.0012	0.0013	0.0013
3.20	0.	0.	0.	0.	0.
3.40	0.	0.	0.	0.	0.
3.60	0.	0.	0.	0.	0.
3.80	0.	0.	0.	0.	0.
4.00	0.	0.	0.	0.	0.
4.50	0.	0.	0.	0.	0.
5.00	0.	0.	0.	0.	0.
5.50	0.	0.	0.	0.	0.
6.00	0.	0.	0.	0.	0.
7.00	0.	0.	0.	0.	0.
8.00	0.	0.	0.	0.	0.
9.00	0.	0.	0.	0.	0.
10.00	0.	0.	0.	0.	0.
12.00	0.	0.	0.	0.	0.
14.00	0.	0.	0.	0.	0.
16.00	0.	0.	0.	0.	0.
18.00	0.	0.	0.	0.	0.

FOR NL-GROUP 1 , THE P(NL,R) ARE AS FOLLOWS

ITERATION= 6

R	
0.	0.
0.02	0.2766
0.04	0.5108
0.06	0.7077
0.08	0.8716
0.10	1.0065
0.12	1.1159
0.14	1.2031
0.16	1.2707
0.18	1.3213
0.20	1.3570
0.25	1.3989
0.30	1.3893
0.35	1.3442
0.40	1.2761
0.45	1.1942
0.50	1.1049
0.55	1.0129
0.60	0.9213
0.70	0.7500
0.80	0.6002
0.90	0.4742
1.00	0.3709
1.10	0.2878
1.20	0.2219
1.30	0.1703
1.40	0.1303
1.60	0.0749
1.80	0.0426
2.00	0.0240

2.20	0.0134
2.40	0.0075
2.60	0.0042
2.80	0.0023
3.00	0.0013
3.20	0.
3.40	0.
3.60	0.
3.80	0.
4.00	0.
4.50	0.
5.00	0.
5.50	0.
6.00	0.
7.00	0.
8.00	0.
9.00	0.
10.00	0.
12.00	0.
14.00	0.
16.00	0.
18.00	0.

FOR NL-GROUP 1 , THE ZO(NL,NL,R) ARE AS FOLLOWS

ITERATION=	1	2	3	4	5
R					
0.	0.	0.	0.	0.	0.
0.02	0.0009	0.0007	0.0008	0.0008	0.0008
0.04	0.0047	0.0040	0.0042	0.0041	0.0041
0.06	0.0134	0.0113	0.0118	0.0117	0.0118
0.08	0.0277	0.0235	0.0245	0.0243	0.0244
0.10	0.0478	0.0406	0.0424	0.0420	0.0421
0.12	0.0734	0.0625	0.0652	0.0645	0.0647
0.14	0.1038	0.0885	0.0923	0.0914	0.0917
0.16	0.1384	0.1181	0.1231	0.1220	0.1223
0.18	0.1762	0.1507	0.1570	0.1555	0.1559
0.20	0.2164	0.1855	0.1931	0.1914	0.1918
0.25	0.3221	0.2779	0.2886	0.2862	0.2869
0.30	0.4283	0.3729	0.3863	0.3832	0.3841
0.35	0.5281	0.4648	0.4801	0.4766	0.4775
0.40	0.6173	0.5498	0.5662	0.5624	0.5634
0.45	0.6944	0.6258	0.6426	0.6388	0.6398
0.50	0.7590	0.6922	0.7087	0.7050	0.7060
0.55	0.8120	0.7490	0.7647	0.7612	0.7621
0.60	0.8546	0.7968	0.8114	0.8081	0.8090
0.70	0.9156	0.8694	0.8814	0.8788	0.8795
0.80	0.9524	0.9177	0.9270	0.9250	0.9256
0.90	0.9737	0.9489	0.9559	0.9544	0.9548
1.00	0.9857	0.9686	0.9736	0.9726	0.9729
1.10	0.9923	0.9809	0.9844	0.9837	0.9839
1.20	0.9959	0.9884	0.9908	0.9903	0.9905
1.30	0.9978	0.9929	0.9946	0.9943	0.9944
1.40	0.9988	0.9957	0.9968	0.9966	0.9967
1.60	0.9997	0.9985	0.9990	0.9989	0.9989
1.80	0.9999	0.9995	0.9997	0.9996	0.9996
2.00	1.0000	0.9998	0.9999	0.9999	0.9999

2.20	1.0000	0.9999	1.0000	1.0000	1.0000
2.40	1.0000	1.0000	1.0000	1.0000	1.0000
2.60	1.0000	1.0000	1.0000	1.0000	1.0000
2.80	1.0000	1.0000	1.0000	1.0000	1.0000
3.00	1.0000	1.0000	1.0000	1.0000	1.0000
3.20	1.0000	1.0000	1.0000	1.0000	1.0000
3.40	1.0000	1.0000	1.0000	1.0000	1.0000
3.60	1.0000	1.0000	1.0000	1.0000	1.0000
3.80	1.0000	1.0000	1.0000	1.0000	1.0000
4.00	1.0000	1.0000	1.0000	1.0000	1.0000
4.50	1.0000	1.0000	1.0000	1.0000	1.0000
5.00	1.0000	1.0000	1.0000	1.0000	1.0000
5.50	1.0000	1.0000	1.0000	1.0000	1.0000
6.00	1.0000	1.0000	1.0000	1.0000	1.0000
7.00	1.0000	1.0000	1.0000	1.0000	1.0000
8.00	1.0000	1.0000	1.0000	1.0000	1.0000
9.00	1.0000	1.0000	1.0000	1.0000	1.0000
10.00	1.0000	1.0000	1.0000	1.0000	1.0000
12.00	1.0000	1.0000	1.0000	1.0000	1.0000
14.00	1.0000	1.0000	1.0000	1.0000	1.0000
16.00	1.0000	1.0000	1.0000	1.0000	1.0000
18.00	1.0000	1.0000	1.0000	1.0000	1.0000

FOR NL-GROUP 1 , THE ZO(NL,NL,R) ARE AS FOLLOWS

ITERATION= 6

R	
0.	0.
0.02	0.0008
0.04	0.0041
0.06	0.0118
0.08	0.0244
0.10	0.0421
0.12	0.0647
0.14	0.0916
0.16	0.1222
0.18	0.1558
0.20	0.1917
0.25	0.2867
0.30	0.3838
0.35	0.4773
0.40	0.5631
0.45	0.6395
0.50	0.7057
0.55	0.7619
0.60	0.8087
0.70	0.8793
0.80	0.9254
0.90	0.9547
1.00	0.9728
1.10	0.9838
1.20	0.9904
1.30	0.9943
1.40	0.9966
1.60	0.9989
1.80	0.9996
2.00	0.9999

2.20	1.0000
2.40	1.0000
2.60	1.0000
2.80	1.0000
3.00	1.0000
3.20	1.0000
3.40	1.0000
3.60	1.0000
3.80	1.0000
4.00	1.0000
4.50	1.0000
5.00	1.0000
5.50	1.0000
6.00	1.0000
7.00	1.0000
8.00	1.0000
9.00	1.0000
10.00	1.0000
12.00	1.0000
14.00	1.0000
16.00	1.0000
18.00	1.0000

FOR NL-GROUP 1 , THE YO(NL,NL,R) ARE AS FOLLOWS

ITERATION=	1	2	3	4	5
R					
0.	0.	0.	0.	0.	0.
0.02	0.0720	0.0661	0.0676	0.0672	0.0673
0.04	0.1431	0.1315	0.1344	0.1337	0.1339
0.06	0.2123	0.1953	0.1995	0.1985	0.1988
0.08	0.2786	0.2566	0.2621	0.2608	0.2612
0.10	0.3414	0.3149	0.3214	0.3199	0.3203
0.12	0.4001	0.3697	0.3772	0.3755	0.3760
0.14	0.4545	0.4209	0.4292	0.4274	0.4279
0.16	0.5046	0.4684	0.4774	0.4753	0.4759
0.18	0.5504	0.5122	0.5217	0.5195	0.5201
0.20	0.5920	0.5524	0.5622	0.5599	0.5606
0.25	0.6859	0.6441	0.6544	0.6521	0.6527
0.30	0.7587	0.7173	0.7276	0.7253	0.7259
0.35	0.8137	0.7747	0.7845	0.7823	0.7829
0.40	0.8545	0.8190	0.8280	0.8260	0.8265
0.45	0.8842	0.8526	0.8607	0.8589	0.8594
0.50	0.9053	0.8778	0.8849	0.8834	0.8838
0.55	0.9199	0.8964	0.9025	0.9012	0.9016
0.60	0.9297	0.9098	0.9151	0.9139	0.9143
0.70	0.9422	0.9286	0.9324	0.9316	0.9318
0.80	0.9460	0.9371	0.9396	0.9391	0.9393
0.90	0.9452	0.9395	0.9412	0.9409	0.9410
1.00	0.9421	0.9385	0.9396	0.9394	0.9394
1.10	0.9377	0.9355	0.9362	0.9361	0.9361
1.20	0.9327	0.9313	0.9318	0.9317	0.9317
1.30	0.9274	0.9266	0.9269	0.9268	0.9269
1.40	0.9220	0.9215	0.9217	0.9216	0.9217
1.60	0.9111	0.9109	0.9110	0.9109	0.9109
1.80	0.9000	0.8999	0.9000	0.8999	0.8999
2.00	0.8889	0.8889	0.8889	0.8889	0.8889

2.20	0.8778	0.8778	0.8778	0.8778	0.8778
2.40	0.8667	0.8667	0.8667	0.8667	0.8667
2.60	0.8556	0.8555	0.8556	0.8556	0.8556
2.80	0.8444	0.8444	0.8444	0.8444	0.8444
3.00	0.8333	0.8333	0.8333	0.8333	0.8333
3.20	0.8222	0.8222	0.8222	0.8222	0.8222
3.40	0.8111	0.8111	0.8111	0.8111	0.8111
3.60	0.8000	0.8000	0.8000	0.8000	0.8000
3.80	0.7889	0.7889	0.7889	0.7889	0.7889
4.00	0.7778	0.7778	0.7778	0.7778	0.7778
4.50	0.7500	0.7500	0.7500	0.7500	0.7500
5.00	0.7222	0.7222	0.7222	0.7222	0.7222
5.50	0.6944	0.6944	0.6944	0.6944	0.6944
6.00	0.6667	0.6667	0.6667	0.6667	0.6667
7.00	0.6111	0.6111	0.6111	0.6111	0.6111
8.00	0.5556	0.5556	0.5556	0.5556	0.5556
9.00	0.5000	0.5000	0.5000	0.5000	0.5000
10.00	0.4444	0.4444	0.4444	0.4444	0.4444
12.00	0.3333	0.3333	0.3333	0.3333	0.3333
14.00	0.2222	0.2222	0.2222	0.2222	0.2222
16.00	0.1111	0.1111	0.1111	0.1111	0.1111
18.00	0.	0.	0.	0.	0.

FOR NL-GROUP 1 , THE Y(NL,R) ARE AS FOLLOWS

ITERATION=	1	2	3	4	5
R					
0.	4.0000	4.0000	4.0000	4.0000	4.0000
0.02	3.9084	3.9328	3.9266	3.9284	3.9279
0.04	3.8169	3.8657	3.8534	3.8568	3.8558
0.06	3.7265	3.7992	3.7808	3.7860	3.7845
0.08	3.6383	3.7342	3.7099	3.7168	3.7148
0.10	3.5532	3.6713	3.6413	3.6498	3.6473
0.12	3.4719	3.6110	3.5756	3.5856	3.5827
0.14	3.3948	3.5536	3.5131	3.5246	3.5212
0.16	3.3222	3.4995	3.4541	3.4669	3.4632
0.18	3.2542	3.4486	3.3986	3.4128	3.4086
0.20	3.0330	3.2693	3.2080	3.2254	3.2203
0.25	2.8827	3.1563	3.0848	3.1051	3.0991
0.30	2.7513	3.0573	2.9768	2.9997	2.9930
0.35	2.6361	2.9712	2.8825	2.9078	2.9004
0.40	2.5341	2.8962	2.8000	2.8274	2.8194
0.45	2.4424	2.8305	2.7271	2.7566	2.7480
0.50	2.3584	2.7722	2.6620	2.6935	2.6843
0.55	2.2803	2.7200	2.6029	2.6364	2.6266
0.60	2.1230	2.6115	2.4815	2.5188	2.5079
0.70	1.9814	2.5227	2.3788	2.4202	2.4080
0.80	1.8496	2.4423	2.2842	2.3297	2.3164
0.90	1.7269	2.3669	2.1947	2.2443	2.2297
1.00	1.6141	2.2948	2.1087	2.1622	2.1465
1.10	1.5123	2.2249	2.0255	2.0827	2.0659
1.20	1.4219	2.1567	1.9452	2.0057	1.9879
1.30	1.3433	2.0901	1.8678	1.9313	1.9127
1.40	1.2142	1.9654	1.7250	1.7933	1.7732
1.60	1.0995	1.8389	1.5838	1.6558	1.6345
1.80	1.0175	1.7199	1.4572	1.5306	1.5088
2.00	0.9601	1.6093	1.3458	1.4187	1.3970

2.20	0.9200	1.5077	1.2496	1.3202	1.2991
2.40	0.8912	1.4155	1.1676	1.2345	1.2143
2.60	0.8696	1.3325	1.0983	1.1606	1.1417
2.80	0.8524	1.2584	1.0400	1.0972	1.0797
3.00	0.8379	1.1925	0.9912	1.0431	1.0271
3.20	0.8248	1.1343	0.9502	0.9969	0.9824
3.40	0.8127	1.0829	0.9157	0.9574	0.9444
3.60	0.8010	1.0378	0.8864	0.9236	0.9119
3.80	0.7896	0.9980	0.8613	0.8944	0.8839
4.00	0.7781	0.9273	0.8235	0.8477	0.8399
4.50	0.7501	0.8495	0.7752	0.7915	0.7862
5.00	0.7222	0.7898	0.7367	0.7478	0.7441
5.50	0.6944	0.7422	0.7035	0.7112	0.7086
6.00	0.6667	0.6904	0.6704	0.6741	0.6728
7.00	0.6111	0.6201	0.6121	0.6133	0.6129
8.00	0.5556	0.5592	0.5558	0.5563	0.5561
9.00	0.5000	0.5018	0.5001	0.5003	0.5002
10.00	0.4444	0.4450	0.4445	0.4445	0.4445
12.00	0.3333	0.3334	0.3333	0.3333	0.3333
14.00	0.2222	0.2222	0.2222	0.2222	0.2222
16.00	0.1111	0.1111	0.1111	0.1111	0.1111
18.00	0.	0.	0.	0.	0.

FOR NL-GROUP 2 , THE P(NL,R) ARE AS FOLLOWS

ITERATION= R	1	2	3	4	5
0.	0.	0.	0.	0.	0.
0.02	0.1043	0.0429	0.0596	0.0549	0.0563
0.04	0.1921	0.0791	0.1100	0.1014	0.1040
0.06	0.2649	0.1095	0.1521	0.1403	0.1438
0.08	0.3239	0.1347	0.1870	0.1725	0.1768
0.10	0.3704	0.1553	0.2153	0.1986	0.2036
0.12	0.4058	0.1719	0.2379	0.2195	0.2250
0.14	0.4309	0.1848	0.2553	0.2357	0.2415
0.16	0.4468	0.1945	0.2681	0.2476	0.2538
0.18	0.4546	0.2014	0.2768	0.2559	0.2622
0.20	0.4549	0.2057	0.2819	0.2608	0.2671
0.25	0.4288	0.2083	0.2825	0.2619	0.2681
0.30	0.3725	0.2010	0.2688	0.2500	0.2558
0.35	0.2949	0.1865	0.2446	0.2286	0.2335
0.40	0.2033	0.1666	0.2127	0.2000	0.2040
0.45	0.1035	0.1427	0.1753	0.1663	0.1692
0.50	0.	0.1160	0.1340	0.1291	0.1308
0.55	-0.1035	0.0873	0.0901	0.0894	0.0899
0.60	-0.2044	0.0573	0.0447	0.0483	0.0475
0.70	-0.3905	-0.0042	-0.0471	-0.0352	-0.0384
0.80	-0.5481	-0.0656	-0.1367	-0.1171	-0.1226
0.90	-0.6731	-0.1249	-0.2212	-0.1948	-0.2023
1.00	-0.7654	-0.1808	-0.2987	-0.2664	-0.2756
1.10	-0.8272	-0.2327	-0.3680	-0.3310	-0.3417
1.20	-0.8620	-0.2801	-0.4287	-0.3881	-0.3999
1.30	-0.8738	-0.3228	-0.4807	-0.4376	-0.4501
1.40	-0.8667	-0.3609	-0.5241	-0.4795	-0.4926
1.60	-0.8115	-0.4248	-0.5884	-0.5440	-0.5570
1.80	-0.7232	-0.4731	-0.6259	-0.5849	-0.5970
2.00	-0.6215	-0.5077	-0.6414	-0.6063	-0.6167

2.20	-0.5194	-0.5313	-0.6393	-0.6119	-0.6203
2.40	-0.4245	-0.5448	-0.6241	-0.6054	-0.6114
2.60	-0.3407	-0.5496	-0.5995	-0.5897	-0.5932
2.80	-0.2694	-0.5474	-0.5683	-0.5673	-0.5684
3.00	-0.2103	-0.5393	-0.5330	-0.5403	-0.5390
3.20	-0.1624	-0.5264	-0.4955	-0.5102	-0.5067
3.40	-0.1242	-0.5099	-0.4571	-0.4784	-0.4730
3.60	-0.0942	-0.4906	-0.4190	-0.4458	-0.4387
3.80	-0.0710	-0.4692	-0.3818	-0.4132	-0.4047
4.00	-0.0531	-0.4463	-0.3461	-0.3812	-0.3715
4.50	-0.0251	-0.3871	-0.2666	-0.3068	-0.2954
5.00	-0.0116	-0.3284	-0.2018	-0.2425	-0.2308
5.50	-0.0052	-0.2738	-0.1509	-0.1892	-0.1780
6.00	-0.0023	-0.2252	-0.1118	-0.1461	-0.1359
7.00	-0.0004	-0.1471	-0.0594	-0.0842	-0.0767
8.00	-0.0001	-0.0931	-0.0309	-0.0474	-0.0422
9.00	-0.0000	-0.0578	-0.0158	-0.0263	-0.0229
10.00	-0.	-0.0356	-0.0082	-0.0146	-0.0125
12.00	-0.	-0.0128	-0.0021	-0.0043	-0.0036
14.00	-0.	-0.0044	-0.0005	-0.0012	-0.0010
16.00	-0.	-0.0015	-0.0001	-0.0003	-0.0003
18.00	0.	0.	0.	0.	0.

FOR NL-GROUP 2 , THE P(NL,R) ARE AS FOLLOWS

ITERATION= 6

R	
0.	0.
0.02	0.0560
0.04	0.1033
0.06	0.1429
0.08	0.1756
0.10	0.2023
0.12	0.2236
0.14	0.2400
0.16	0.2521
0.18	0.2605
0.20	0.2655
0.25	0.2665
0.30	0.2543
0.35	0.2322
0.40	0.2030
0.45	0.1685
0.50	0.1304
0.55	0.0898
0.60	0.0478
0.70	-0.0375
0.80	-0.1211
0.90	-0.2002
1.00	-0.2731
1.10	-0.3388
1.20	-0.3967
1.30	-0.4468
1.40	-0.4891
1.60	-0.5537
1.80	-0.5940
2.00	-0.6142

2.20	-0.6183
2.40	-0.6099
2.60	-0.5923
2.80	-0.5681
3.00	-0.5393
3.20	-0.5076
3.40	-0.4744
3.60	-0.4406
3.80	-0.4069
4.00	-0.3741
4.50	-0.2984
5.00	-0.2339
5.50	-0.1809
6.00	-0.1386
7.00	-0.0786
8.00	-0.0435
9.00	-0.0238
10.00	-0.0131
12.00	-0.0038
14.00	-0.0011
16.00	-0.0003
18.00	0.

FOR NL-GROUP 2 , THE ZO(NL,NL,R) ARE AS FOLLOWS

ITERATION=	1	2	3	4	5
R					
0.	0.	0.	0.	0.	0.
0.02	0.0001	0.0000	0.0000	0.0000	0.0000
0.04	0.0006	0.0001	0.0002	0.0002	0.0002
0.06	0.0017	0.0003	0.0005	0.0005	0.0005
0.08	0.0034	0.0006	0.0011	0.0010	0.0010
0.10	0.0058	0.0010	0.0019	0.0016	0.0017
0.12	0.0088	0.0015	0.0030	0.0025	0.0026
0.14	0.0123	0.0022	0.0042	0.0036	0.0037
0.16	0.0162	0.0029	0.0056	0.0047	0.0050
0.18	0.0203	0.0037	0.0070	0.0060	0.0063
0.20	0.0244	0.0045	0.0086	0.0073	0.0077
0.25	0.0342	0.0067	0.0126	0.0107	0.0113
0.30	0.0422	0.0087	0.0164	0.0140	0.0147
0.35	0.0479	0.0106	0.0197	0.0169	0.0177
0.40	0.0511	0.0122	0.0223	0.0192	0.0201
0.45	0.0524	0.0134	0.0242	0.0209	0.0219
0.50	0.0527	0.0142	0.0254	0.0220	0.0230
0.55	0.0529	0.0148	0.0261	0.0226	0.0236
0.60	0.0542	0.0150	0.0263	0.0229	0.0239
0.70	0.0640	0.0152	0.0265	0.0230	0.0241
0.80	0.0866	0.0154	0.0276	0.0238	0.0249
0.90	0.1243	0.0164	0.0310	0.0264	0.0277
1.00	0.1762	0.0188	0.0379	0.0318	0.0336
1.10	0.2397	0.0232	0.0491	0.0408	0.0432
1.20	0.3111	0.0298	0.0651	0.0539	0.0570
1.30	0.3864	0.0389	0.0858	0.0710	0.0752
1.40	0.4622	0.0507	0.1111	0.0920	0.0974
1.60	0.6031	0.0817	0.1732	0.1446	0.1527
1.80	0.7213	0.1222	0.2470	0.2084	0.2194
2.00	0.8123	0.1703	0.3273	0.2794	0.2931

2.20	0.8779	0.2243	0.4093	0.3536	0.3696
2.40	0.9229	0.2822	0.4891	0.4277	0.4454
2.60	0.9525	0.3421	0.5640	0.4991	0.5180
2.80	0.9714	0.4023	0.6323	0.5661	0.5855
3.00	0.9830	0.4613	0.6930	0.6274	0.6468
3.20	0.9901	0.5181	0.7459	0.6827	0.7016
3.40	0.9943	0.5718	0.7914	0.7316	0.7496
3.60	0.9967	0.6219	0.8298	0.7744	0.7912
3.80	0.9981	0.6680	0.8620	0.8113	0.8269
4.00	0.9989	0.7099	0.8885	0.8429	0.8571
4.50	0.9998	0.7972	0.9362	0.9028	0.9134
5.00	0.9999	0.8616	0.9642	0.9410	0.9485
5.50	1.0000	0.9073	0.9801	0.9647	0.9698
6.00	1.0000	0.9387	0.9889	0.9789	0.9823
7.00	1.0000	0.9749	0.9969	0.9932	0.9945
8.00	1.0000	0.9900	0.9992	0.9978	0.9983
9.00	1.0000	0.9960	0.9998	0.9993	0.9995
10.00	1.0000	0.9984	0.9999	0.9997	0.9998
12.00	1.0000	0.9998	1.0000	1.0000	1.0000
14.00	1.0000	1.0000	1.0000	1.0000	1.0000
16.00	1.0000	1.0000	1.0000	1.0000	1.0000
18.00	1.0000	1.0000	1.0000	1.0000	1.0000

FOR NL-GROUP 2 , THE ZO(NL,NL,R) ARE AS FOLLOWS

ITERATION= 6

R	
0.	0.
0.02	0.0000
0.04	0.0002
0.06	0.0005
0.08	0.0010
0.10	0.0017
0.12	0.0026
0.14	0.0037
0.16	0.0049
0.18	0.0062
0.20	0.0076
0.25	0.0111
0.30	0.0145
0.35	0.0175
0.40	0.0199
0.45	0.0216
0.50	0.0227
0.55	0.0234
0.60	0.0236
0.70	0.0238
0.80	0.0246
0.90	0.0274
1.00	0.0331
1.10	0.0426
1.20	0.0562
1.30	0.0740
1.40	0.0960
1.60	0.1505
1.80	0.2165
2.00	0.2895

2.20	0.3654
2.40	0.4408
2.60	0.5131
2.80	0.5805
3.00	0.6419
3.20	0.6967
3.40	0.7450
3.60	0.7869
3.80	0.8229
4.00	0.8534
4.50	0.9107
5.00	0.9466
5.50	0.9685
6.00	0.9815
7.00	0.9942
8.00	0.9982
9.00	0.9994
10.00	0.9998
12.00	1.0000
14.00	1.0000
16.00	1.0000
18.00	1.0000

FOR NL-GROUP 2 , THE YO(NL,NL,R) ARE AS FOLLOWS

ITERATION=	1	2	3	4	5
R					
0.	0.	0.	0.	0.	0.
0.02	0.0176	0.0069	0.0095	0.0088	0.0090
0.04	0.0351	0.0137	0.0191	0.0175	0.0179
0.06	0.0523	0.0205	0.0285	0.0261	0.0268
0.08	0.0692	0.0272	0.0378	0.0347	0.0356
0.10	0.0856	0.0339	0.0470	0.0431	0.0443
0.12	0.1016	0.0405	0.0560	0.0514	0.0528
0.14	0.1171	0.0469	0.0649	0.0596	0.0611
0.16	0.1320	0.0533	0.0735	0.0676	0.0693
0.18	0.1465	0.0596	0.0820	0.0754	0.0774
0.20	0.1605	0.0659	0.0904	0.0832	0.0853
0.25	0.1946	0.0812	0.1108	0.1021	0.1047
0.30	0.2266	0.0961	0.1304	0.1204	0.1233
0.35	0.2574	0.1107	0.1494	0.1381	0.1414
0.40	0.2873	0.1250	0.1680	0.1554	0.1591
0.45	0.3168	0.1391	0.1862	0.1725	0.1765
0.50	0.3462	0.1530	0.2042	0.1893	0.1937
0.55	0.3756	0.1669	0.2221	0.2060	0.2107
0.60	0.4049	0.1807	0.2399	0.2227	0.2277
0.70	0.4633	0.2083	0.2755	0.2560	0.2617
0.80	0.5204	0.2359	0.3110	0.2893	0.2957
0.90	0.5746	0.2635	0.3465	0.3225	0.3295
1.00	0.6247	0.2910	0.3815	0.3554	0.3630
1.10	0.6695	0.3182	0.4159	0.3877	0.3960
1.20	0.7086	0.3450	0.4492	0.4193	0.4281
1.30	0.7417	0.3713	0.4812	0.4497	0.4590
1.40	0.7690	0.3968	0.5117	0.4789	0.4885
1.60	0.8129	0.4463	0.5689	0.5341	0.5444
1.80	0.8391	0.4918	0.6183	0.5828	0.5933
2.00	0.8522	0.5329	0.6596	0.6244	0.6349

2.20	0.8562	0.5692	0.6928	0.6589	0.6691
2.40	0.8542	0.6005	0.7186	0.6867	0.6963
2.60	0.8485	0.6271	0.7377	0.7083	0.7172
2.80	0.8405	0.6490	0.7511	0.7243	0.7325
3.00	0.8311	0.6666	0.7596	0.7356	0.7430
3.20	0.8210	0.6803	0.7640	0.7429	0.7494
3.40	0.8104	0.6904	0.7652	0.7466	0.7524
3.60	0.7996	0.6974	0.7636	0.7475	0.7526
3.80	0.7886	0.7016	0.7599	0.7460	0.7504
4.00	0.7776	0.7034	0.7546	0.7426	0.7464
4.50	0.7500	0.7025	0.7378	0.7300	0.7326
5.00	0.7222	0.6920	0.7158	0.7108	0.7125
5.50	0.6944	0.6751	0.6909	0.6878	0.6889
6.00	0.6667	0.6539	0.6647	0.6627	0.6634
7.00	0.6111	0.6065	0.6106	0.6100	0.6102
8.00	0.5556	0.5539	0.5554	0.5552	0.5553
9.00	0.5000	0.4993	0.5000	0.4999	0.4999
10.00	0.4444	0.4441	0.4444	0.4444	0.4444
12.00	0.3333	0.3333	0.3333	0.3333	0.3333
14.00	0.2222	0.2222	0.2222	0.2222	0.2222
16.00	0.1111	0.1111	0.1111	0.1111	0.1111
18.00	0.	0.	0.	0.	0.

FOR NL-GROUP 2 , THE Y(NL,R) ARE AS FOLLOWS

ITERATION=	1	2	3	4	5
R					
0.	4.0000	4.0000	4.0000	4.0000	4.0000
0.02	3.8540	3.8735	3.8686	3.8699	3.8695
0.04	3.7089	3.7478	3.7380	3.7406	3.7399
0.06	3.5665	3.6244	3.6098	3.6136	3.6125
0.08	3.4288	3.5048	3.4857	3.4907	3.4892
0.10	3.2975	3.3903	3.3669	3.3730	3.3712
0.12	3.1734	3.2817	3.2544	3.2615	3.2595
0.14	3.0573	3.1797	3.1487	3.1568	3.1545
0.16	2.9496	3.0844	3.0502	3.0592	3.0566
0.18	2.8503	2.9960	2.9589	2.9687	2.9659
0.20	2.6016	2.7828	2.7362	2.7486	2.7450
0.25	2.3914	2.5934	2.5411	2.5551	2.5511
0.30	2.2192	2.4361	2.3796	2.3948	2.3904
0.35	2.0798	2.3072	2.2475	2.2636	2.2589
0.40	1.9669	2.2022	2.1400	2.1569	2.1520
0.45	1.8751	2.1169	2.0526	2.0702	2.0651
0.50	1.7994	2.0474	1.9812	1.9994	1.9941
0.55	1.7359	1.9905	1.9224	1.9412	1.9357
0.60	1.5981	1.8825	1.8063	1.8276	1.8214
0.70	1.5026	1.8024	1.7219	1.7446	1.7379
0.80	1.4240	1.7411	1.6556	1.6799	1.6728
0.90	1.3563	1.6909	1.6000	1.6259	1.6183
1.00	1.2967	1.6473	1.5506	1.5782	1.5701
1.10	1.2441	1.6076	1.5052	1.5344	1.5258
1.20	1.1978	1.5703	1.4626	1.4933	1.4843
1.30	1.1576	1.5348	1.4222	1.4542	1.4448
1.40	1.0612	1.4407	1.3150	1.3505	1.3400
1.60	1.0013	1.3743	1.2418	1.2790	1.2680
1.80	0.9566	1.3118	1.1756	1.2135	1.2022
2.00	0.9234	1.2533	1.1166	1.1543	1.1430

2.20	0.8983	1.1992	1.0647	1.1013	1.0903
2.40	0.8787	1.1494	1.0195	1.0545	1.0439
2.60	0.8625	1.1040	0.9805	1.0133	1.0033
2.80	0.8485	1.0629	0.9467	0.9771	0.9678
3.00	0.8357	1.0258	0.9174	0.9454	0.9368
3.20	0.8236	0.9923	0.8920	0.9175	0.9096
3.40	0.8120	0.9622	0.8697	0.8929	0.8857
3.60	0.8006	0.9352	0.8500	0.8711	0.8645
3.80	0.7893	0.9107	0.8323	0.8515	0.8455
4.00	0.7779	0.8529	0.8003	0.8125	0.8086
4.50	0.7500	0.8021	0.7630	0.7716	0.7688
5.00	0.7222	0.7596	0.7303	0.7364	0.7344
5.50	0.6944	0.7228	0.7000	0.7046	0.7031
6.00	0.6667	0.6777	0.6684	0.6701	0.6695
7.00	0.6111	0.6155	0.6116	0.6122	0.6120
8.00	0.5556	0.5575	0.5557	0.5559	0.5558
9.00	0.5000	0.5011	0.5001	0.5002	0.5001
10.00	0.4444	0.4447	0.4444	0.4445	0.4445
12.00	0.3333	0.3334	0.3333	0.3333	0.3333
14.00	0.2222	0.2222	0.2222	0.2222	0.2222
16.00	0.1111	0.1111	0.1111	0.1111	0.1111
18.00	0.	0.	0.	0.	0.

THE Y(R) ARE AS FOLLOWS

ITERATION=	1	2	3	4	5
R					
0.02	4.0000	4.0000	4.0000	4.0000	4.0000
0.04	3.8364	3.8667	3.8591	3.8611	3.8605
0.06	3.6738	3.7342	3.7190	3.7231	3.7219
0.08	3.5142	3.6039	3.5813	3.5875	3.5857
0.10	3.3596	3.4776	3.4479	3.4560	3.4536
0.12	3.2118	3.3564	3.3199	3.3298	3.3270
0.14	3.0718	3.2412	3.1983	3.2101	3.2067
0.16	2.9403	3.1327	3.0838	3.0972	3.0933
0.18	2.8176	3.0311	2.9767	2.9916	2.9873
0.20	2.7038	2.9364	2.8769	2.8932	2.8885
0.25	2.4410	2.7169	2.6458	2.6654	2.6597
0.30	2.1968	2.5122	2.4303	2.4530	2.4464
0.35	1.9926	2.3400	2.2492	2.2744	2.2671
0.40	1.8224	2.1965	2.0980	2.1255	2.1175
0.45	1.6796	2.0772	1.9720	2.0015	1.9929
0.50	1.5582	1.9778	1.8664	1.8977	1.8886
0.55	1.4532	1.8944	1.7770	1.8101	1.8005
0.60	1.3604	1.8236	1.7003	1.7352	1.7250
0.70	1.1932	1.7017	1.5664	1.6049	1.5936
0.80	1.0392	1.5940	1.4464	1.4886	1.4762
0.90	0.9036	1.5051	1.3446	1.3906	1.3771
1.00	0.7817	1.4274	1.2535	1.3034	1.2888
1.10	0.6721	1.3563	1.1691	1.2228	1.2071
1.20	0.5746	1.2894	1.0893	1.1467	1.1298
1.30	0.4892	1.2253	1.0133	1.0740	1.0562
1.40	0.4159	1.1635	0.9409	1.0045	0.9858
1.60	0.2922	1.0439	0.8034	0.8716	0.8515
1.80	0.1884	0.9280	0.6729	0.7448	0.7236
2.00	0.1175	0.8199	0.5572	0.6307	0.6089
2.20	0.0712	0.7204	0.4570	0.5298	0.5081

2.40	0.0422	0.6300	0.3719	0.4424	0.4213
2.60	0.0245	0.5489	0.3009	0.3678	0.3477
2.80	0.0140	0.4770	0.2427	0.3050	0.2861
3.00	0.0080	0.4139	0.1956	0.2528	0.2353
3.20	0.0045	0.3592	0.1579	0.2097	0.1938
3.40	0.0026	0.3120	0.1280	0.1747	0.1602
3.60	0.0016	0.2718	0.1046	0.1463	0.1333
3.80	0.0010	0.2378	0.0864	0.1236	0.1119
4.00	0.0007	0.2092	0.0724	0.1055	0.0950
4.50	0.0003	0.1495	0.0457	0.0699	0.0621
5.00	0.0001	0.0995	0.0252	0.0415	0.0362
5.50	0.0000	0.0676	0.0145	0.0256	0.0219
6.00	0.	0.0477	0.0091	0.0168	0.0142
7.00	0.	0.0237	0.0037	0.0074	0.0061
8.00	0.	0.0090	0.0009	0.0022	0.0018
9.00	0.	0.0037	0.0003	0.0007	0.0005
10.00	0.	0.0018	0.0001	0.0003	0.0002
12.00	0.	0.0005	0.0000	0.0001	0.0001
14.00	0.	0.0001	0.	0.0000	0.
16.00	0.	0.0000	0.	0.	0.
18.00	0.	0.	0.	0.	0.

THE Z(R) ARE AS FOLLOWS

ITERATION=	1	2	3	4	5
R					
0.	4.0000	4.0000	4.0000	4.0000	4.0000
0.02	3.9980	3.9985	3.9984	3.9984	3.9984
0.04	3.9894	3.9918	3.9913	3.9914	3.9914
0.06	3.9699	3.9767	3.9752	3.9756	3.9755
0.08	3.9378	3.9518	3.9486	3.9494	3.9492
0.10	3.8927	3.9167	3.9113	3.9127	3.9123
0.12	3.8355	3.8720	3.8637	3.8658	3.8652
0.14	3.7677	3.8186	3.8070	3.8100	3.8092
0.16	3.6909	3.7579	3.7426	3.7465	3.7454
0.18	3.6071	3.6912	3.6719	3.6769	3.6755
0.20	3.5183	3.6199	3.5966	3.6026	3.6009
0.25	3.2875	3.4308	3.3975	3.4061	3.4037
0.30	3.0589	3.2366	3.1946	3.2054	3.2024
0.35	2.8481	3.0492	3.0004	3.0130	3.0095
0.40	2.6631	2.8761	2.8230	2.8367	2.8328
0.45	2.5065	2.7215	2.6664	2.6807	2.6766
0.50	2.3767	2.5870	2.5317	2.5461	2.5420
0.55	2.2702	2.4724	2.4184	2.4324	2.4284
0.60	2.1822	2.3764	2.3246	2.3381	2.3342
0.70	2.0408	2.2307	2.1841	2.1963	2.1928
0.80	1.9220	2.1337	2.0907	2.1023	2.0990
0.90	1.8040	2.0693	2.0263	2.0384	2.0349
1.00	1.6761	2.0251	1.9770	1.9911	1.9871
1.10	1.5358	1.9919	1.9330	1.9509	1.9458
1.20	1.3859	1.9636	1.8882	1.9116	1.9050
1.30	1.2315	1.9362	1.8392	1.8695	1.8609
1.40	1.0780	1.9073	1.7842	1.8227	1.8118
1.60	0.7943	1.8395	1.6557	1.7130	1.6967
1.80	0.5575	1.7567	1.5067	1.5839	1.5619
2.00	0.3755	1.6597	1.3456	1.4414	1.4141

2.20	0.2443	1.5515	1.1814	1.2929	1.2609
2.40	0.1543	1.4356	1.0218	1.1446	1.1092
2.60	0.0950	1.3158	0.8720	1.0018	0.9640
2.80	0.0573	1.1954	0.7355	0.8678	0.8290
3.00	0.0339	1.0773	0.6140	0.7451	0.7063
3.20	0.0198	0.9637	0.5081	0.6347	0.5969
3.40	0.0114	0.8563	0.4172	0.5368	0.5008
3.60	0.0066	0.7562	0.3403	0.4513	0.4175
3.80	0.0038	0.6640	0.2760	0.3774	0.3462
4.00	0.0022	0.5802	0.2229	0.3142	0.2859
4.50	0.0005	0.4056	0.1275	0.1945	0.1732
5.00	0.0001	0.2768	0.0716	0.1180	0.1029
5.50	0.0000	0.1854	0.0398	0.0707	0.0604
6.00	0.0000	0.1225	0.0222	0.0421	0.0354
7.00	0.	0.0502	0.0062	0.0137	0.0110
8.00	0.	0.0199	0.0017	0.0043	0.0034
9.00	0.	0.0079	0.0005	0.0014	0.0010
10.00	0.	0.0033	0.0001	0.0005	0.0004
12.00	0.	0.0004	0.0000	0.0000	0.0000
14.00	0.	0.0000	0.	0.	0.
16.00	0.	0.	0.	0.	0.
18.00	0.	0.	0.	0.	0.

THE Z(R) ARE AS FOLLOWS

ITERATION= 6

R	
0.	4.0000
0.02	3.9984
0.04	3.9914
0.06	3.9755
0.08	3.9493
0.10	3.9124
0.12	3.8654
0.14	3.8094
0.16	3.7457
0.18	3.6759
0.20	3.6014
0.25	3.4044
0.30	3.2032
0.35	3.0105
0.40	2.8339
0.45	2.6777
0.50	2.5431
0.55	2.4295
0.60	2.3353
0.70	2.1938
0.80	2.0999
0.90	2.0359
1.00	1.9882
1.10	1.9472
1.20	1.9068
1.30	1.8633
1.40	1.8148
1.60	1.7011
1.80	1.5677
2.00	1.4213

2.20	1.2692
2.40	1.1183
2.60	0.9737
2.80	0.8390
3.00	0.7163
3.20	0.6065
3.40	0.5100
3.60	0.4262
3.80	0.3542
4.00	0.2931
4.50	0.1786
5.00	0.1067
5.50	0.0630
6.00	0.0371
7.00	0.0117
8.00	0.0036
9.00	0.0011
10.00	0.0004
12.00	0.0000
14.00	0.
16.00	0.
18.00	0.